Neophytadiene

Inchi: InChI=1S/C20H38/c1-7-18(4)12-9-14-20(6)16-10-15-19(5)13-8-11-17(2)3/h7,17,19-20H,1
InchiKey: NIDGCIPAMWNKOA-UHFFFAOYSA-N
Formula: C20H38
SMILES: C=CC(=C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 278.52
CAS: 504-96-1

Physical Properties

Property code	Value	Unit	Source
gf	277.33	kJ/mol	Joback Method
hf	-230.90	kJ/mol	Joback Method
hfus	33.12	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	7.168		Crippen Method
mcvol	284.060	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	1836.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1844.10		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1840.60		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1806.00		NIST Webbook

rinpol	1837.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1840.60		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1817.00		NIST Webbook
rinpol	1838.00		NIST Webbook
ripol	1933.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1912.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1922.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1931.00		NIST Webbook
ripol	1931.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1910.00		NIST Webbook
tb	648.92	K	Joback Method
tc	820.03	K	Joback Method
tf	252.68	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.06	J/mol×K	648.92	Joback Method
cpg	815.13	J/mol×K	677.44	Joback Method
cpg	835.25	J/mol×K	705.96	Joback Method
cpg	854.45	J/mol×K	734.48	Joback Method
cpg	872.75	J/mol×K	763.00	Joback Method
cpg	890.21	J/mol×K	791.51	Joback Method
cpg	906.86	J/mol×K	820.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C504961&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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