Neophytadiene, isomer II

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

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	1841.00		NIST Webbook
rinpol	1841.00		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=R640010&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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