

Neophytadiene isomer # 2

Other names:	Neophytadiene isomer # 2
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,1,2,4,5,6,8,10,11,12,13,14,15,16,18,20H,3H,4H
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
af	0.7045		Cheméo Relay (1.0)
hfus	33.12	kJ/mol	Joback Method
hvap	82.39	kJ/mol	Cheméo Relay (1.0)
logp	7.168		Crippen Method
mcvol	284.060	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	1881.00		NIST Webbook
tb	578.47	K	Cheméo Relay (1.0)
tc	737.92	K	Cheméo Relay (1.0)
tf	225.01	K	Cheméo Relay (1.0)
vc	1.039	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R430734&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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