1-Methyl-4-(1-methylethyl)-3-[1-methyl-1-(4-methy

Other names: 3-[1,5-Dimethyl-1-(4-methyl-pentyl)-heptyl]-4-isopropyl-1-methyl-cyclohexene
Inchi: InChI=1S/C25H48/c1-9-21(6)13-11-17-25(8,16-10-12-19(2)3)24-18-22(7)14-15-23(24)20
InchiKey: BSFSYBSOZFHRHQ-UHFFFAOYSA-N
Formula: C25H48
SMILES: CCC(C)CCCC(C)(CCCC(C)C)C1C=C(C)CCC1C(C)C
Mol. weight [g/mol]: 348.65

Physical Properties

Property code	Value	Unit	Source
gf	192.21	kJ/mol	Joback Method
hf	-503.63	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	69.86	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	8.664		Crippen Method
mcvol	347.950	ml/mol	McGowan Method
pc	874.28	kPa	Joback Method
rinpol	2078.00		NIST Webbook
rinpol	2087.00		NIST Webbook
tb	785.87	K	Joback Method
tc	977.85	K	Joback Method
tf	345.35	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.98	J/mol×K	785.87	Joback Method
cpg	1154.56	J/mol×K	817.87	Joback Method
cpg	1177.72	J/mol×K	849.86	Joback Method
cpg	1199.55	J/mol×K	881.86	Joback Method
cpg	1220.11	J/mol×K	913.86	Joback Method
cpg	1239.44	J/mol×K	945.85	Joback Method
cpg	1257.63	J/mol×K	977.85	Joback Method

dvisc	0.0038806	Pa×s	345.35	Joback Method
dvisc	0.0009617	Pa×s	418.77	Joback Method
dvisc	0.0003613	Pa×s	492.19	Joback Method
dvisc	0.0001751	Pa×s	565.61	Joback Method
dvisc	0.0001002	Pa×s	639.03	Joback Method
dvisc	0.0000643	Pa×s	712.45	Joback Method
dvisc	0.0000449	Pa×s	785.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370414&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
dvisc:	Dynamic viscosity
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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