10-Demethylsqualene

Inchi: InChI=1S/C29H48/c1-25(2)17-14-21-27(5)19-12-10-8-9-11-13-20-28(6)23-16-24-29(7)22
InchiKey: BBCQGYMUMKNTQE-BAIGTOHMSA-N
Formula: C29H48
SMILES: CC(C)=CCCC(C)=CCCC=CCCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 396.69

Physical Properties

Property code	Value	Unit	Source
gf	631.87	kJ/mol	Joback Method
hf	12.48	kJ/mol	Joback Method
hfus	65.53	kJ/mol	Joback Method
hvap	80.30	kJ/mol	Joback Method
log10ws	-11.08		Crippen Method
logp	10.215		Crippen Method
mcvol	393.670	ml/mol	McGowan Method
pc	744.48	kPa	Joback Method
rinpol	2813.00		NIST Webbook
rinpol	2813.00		NIST Webbook
rinpol	2859.00		NIST Webbook
rinpol	2830.00		NIST Webbook
rinpol	2830.00		NIST Webbook
tb	887.28	K	Joback Method
tc	1089.10	K	Joback Method
tf	316.31	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1257.00	J/mol×K	887.28	Joback Method
cpg	1279.79	J/mol×K	920.92	Joback Method
cpg	1301.81	J/mol×K	954.55	Joback Method
cpg	1323.22	J/mol×K	988.19	Joback Method
cpg	1344.16	J/mol×K	1021.83	Joback Method

cpg	1364.77	J/mol×K	1055.46	Joback Method
cpg	1385.20	J/mol×K	1089.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R615257&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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