Grandisol

Other names:	Cyclobutaneethanol, 1-methyl-2-(1-methylethenyl)-, (1R-cis)- Cyclobutaneethanol, 2-isopropenyl-1-methyl-, cis-(+)- (+)-Grandisol cis-2-Isopropenyl-1-methylcyclobutaneethanol 2-(2-Isopropenyl-1-methylcyclobutyl)ethanol)-, (1R,2S)- (+)-cis-2-Isopropenyl-1-methylcyclobutaneethanol Grandlure I Cyclobutaneethanol, 1-methyl-2-(1-methylethenyl)-, (1R,2S)-
Inchi:	InChI=1S/C10H18O/c1-8(2)9-4-5-10(9,3)6-7-11/h9,11H,1,4-7H2,2-3H3/t9-,10-/m1/s1
InchiKey:	SJKPJXGGNKMRPD-UWVGGRQHSA-N
Formula:	C10H18O
SMILES:	C=C(C)[C@H]1CC[C@]1(C)CCO
Mol. weight [g/mol]:	154.25

Physical Properties

Property code	Value	Unit	Source
hfus	13.96	kJ/mol	Joback Method
ie	8.96	eV	Cheméo Relay (1.0)
logp	2.361		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
rinpol	1200.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook
ripol	1865.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.60	J/mol×K	523.52	Joback Method
cpg	363.16	J/mol×K	554.70	Joback Method

cpg	376.87	J/mol×K	585.88	Joback Method
cpg	389.82	J/mol×K	617.07	Joback Method
cpg	402.10	J/mol×K	648.25	Joback Method
cpg	413.80	J/mol×K	679.43	Joback Method
cpg	425.00	J/mol×K	710.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C26532229&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices