Cyclobutaneethanol, 1-methyl-2-(1-methylethenyl)-, trans-

Other names:	Cyclobutaneethanol, 2-isopropenyl-1-methyl-, stereoisomer
	Fragranol
	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-/m0/s1
InchiKey:	SJKPJXGGNKMRPD-UWVGGRQHSA-N
Formula:	C10H18O
SMILES:	C=C(C)C1CCC1(C)CCO
Mol. weight [g/mol]:	154.25
CAS:	30346-21-5

Physical Properties

Property code	Value	Unit	Source
gf	11.24	kJ/mol	Joback Method
hf	-224.78	kJ/mol	Joback Method
hfus	13.96	kJ/mol	Joback Method
hvap	52.57	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.361		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1196.00		NIST Webbook
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	1213.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1212.00		NIST Webbook

rinpol	1221.60		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1200.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1769.00		NIST Webbook
tb	523.52	K	Joback Method
tc	710.61	K	Joback Method
tf	281.64	K	Joback Method
vc	0.542	m3/kmol	Joback Method

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26532229&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume