Ethanol, 2-(3,3-dimethylcyclohexylidene)-, (Z)-

Other names:	(Z)-2-(3,3-Dimethylcyclohexylidene)ethanol
	(2Z)-2-(3,3-Dimethylcyclohexylidene)ethanol
	cis-3,3-dimethyl-«delta»1-«beta»-cyclohexanethanol
	Grandlure II
	Ethanol, 2-(3,3-dimethylcyclohexylidene)-, (2Z)-
Inchi:	InChI=1S/C10H18O/c1-10(2)6-3-4-9(8-10)5-7-11/h5,11H,3-4,6-8H2,1-2H3/b9-5-
InchiKey:	SHYLMMBHTKLAJS-UITAMQMPSA-N
Formula:	C10H18O
SMILES:	CC1(C)CCCC(=CCO)C1
Mol. weight [g/mol]:	154.25
CAS:	26532-23-0

Physical Properties

Property code	Value	Unit	Source
gf	-39.08	kJ/mol	Joback Method
hf	-256.37	kJ/mol	Joback Method
hfus	11.60	kJ/mol	Joback Method
hvap	54.60	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.505		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1225.00		NIST Webbook
ripol	1865.00		NIST Webbook
tb	546.81	K	Joback Method
tc	746.23	K	Joback Method
tf	304.92	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.74	J/mol×K	546.81	Joback Method
cpg	364.83	J/mol×K	580.05	Joback Method

cpg	379.05	J/mol×K	613.28	Joback Method
cpg	392.50	J/mol×K	646.52	Joback Method
cpg	405.27	J/mol×K	679.76	Joback Method
cpg	417.46	J/mol×K	712.99	Joback Method
cpg	429.16	J/mol×K	746.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26532230&Units=SI

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