Bicyclo(3.1.1)heptane-2,3-diol, 2,6,6-trimethyl-

Other names:	DHS activator
	Ethylene glycol ether of pinene
	2,3-Pinanediol
	Pinanediol
Inchi:	InChI=1S/C10H18O2/c1-9(2)6-4-7(9)10(3,12)8(11)5-6/h6-8,11-12H,4-5H2,1-3H3
InchiKey:	MOILFCKRQFQVFS-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CC1(C)C2CC(O)C(C)(O)C1C2
Mol. weight [g/mol]:	170.25
CAS:	53404-49-2

Physical Properties

Property code	Value	Unit	Source
gf	-165.03	kJ/mol	Joback Method
hf	-445.29	kJ/mol	Joback Method
hfus	14.62	kJ/mol	Joback Method
hvap	67.98	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.164		Crippen Method
mcvol	141.780	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	1244.00		NIST Webbook
tb	616.78	K	Joback Method
tc	805.96	K	Joback Method
tf	391.54	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.70	J/mol×K	616.78	Joback Method
cpg	427.85	J/mol×K	648.31	Joback Method
cpg	440.40	J/mol×K	679.84	Joback Method
cpg	452.49	J/mol×K	711.37	Joback Method

cpg	464.29	J/mol×K	742.90	Joback Method
cpg	475.94	J/mol×K	774.43	Joback Method
cpg	487.59	J/mol×K	805.96	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=C53404492&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume