(Z)-3,3-dimethylcyclohexane-«DELTA»1,«beta»-et acetate

Inchi: InChI=1S/C12H20O2/c1-12(2)8-4-6-10(9-12)5-3-7-11(13)14/h5H,3-4,6-9H2,1-2H3,(H,13,

InchiKey: MOVMOZAHZNEFET-YHYXMXQVSA-N

Formula: C12H20O2

SMILES: CC1(C)CCCC(=CCCC(=O)O)C1

Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-151.16	kJ/mol	Joback Method
hf	-410.23	kJ/mol	Joback Method
hfus	18.38	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.378		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1325.00		NIST Webbook
rinpol	1325.00		NIST Webbook
tb	646.44	K	Joback Method
tc	847.77	K	Joback Method
tf	377.39	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.07	J/mol×K	646.44	Joback Method
cpg	484.04	J/mol×K	680.00	Joback Method
cpg	498.28	J/mol×K	713.55	Joback Method
cpg	511.90	J/mol×K	747.11	Joback Method
cpg	524.99	J/mol×K	780.66	Joback Method
cpg	537.65	J/mol×K	814.22	Joback Method
cpg	549.98	J/mol×K	847.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R216489&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

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

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