(Z)-3,3-dimethylcyclohexane-«DELTA»1,«alpha»-a acid

Inchi: InChI=1S/C10H16O2/c1-10(2)5-3-4-8(7-10)6-9(11)12/h6H,3-5,7H2,1-2H3,(H,11,12)/b8-6

InchiKey: LKJIOHQBVGRPCO-VURMDHGXSA-N

Formula: C10H16O2

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

Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-168.00	kJ/mol	Joback Method
hf	-368.95	kJ/mol	Joback Method
hfus	13.20	kJ/mol	Joback Method
hvap	61.34	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.598		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
tb	600.68	K	Joback Method
tc	807.94	K	Joback Method
tf	354.85	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.08	J/mol×K	600.68	Joback Method
cpg	382.81	J/mol×K	635.22	Joback Method
cpg	395.77	J/mol×K	669.77	Joback Method
cpg	408.08	J/mol×K	704.31	Joback Method
cpg	419.84	J/mol×K	738.85	Joback Method
cpg	431.14	J/mol×K	773.39	Joback Method
cpg	442.09	J/mol×K	807.94	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=R216474&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

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