ethyl (Z)-3,3-dimethyl~yclohexane-«DELTA»1,«alpha»-a

Inchi: InChI=1S/C12H20O2/c1-4-14-11(13)8-10-6-5-7-12(2,3)9-10/h8H,4-7,9H2,1-3H3/b10-8-

InchiKey: BKHNGPZOPOPDCJ-NTMALXAHSA-N

Formula: C12H20O2

SMILES: CCOC(=O)C=C1CCCC(C)(C)C1

Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-119.34	kJ/mol	Joback Method
hf	-390.22	kJ/mol	Joback Method
hfus	15.48	kJ/mol	Joback Method
hvap	51.53	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.076		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1328.00		NIST Webbook
tb	576.68	K	Joback Method
tc	790.27	K	Joback Method
tf	338.80	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.97	J/mol×K	576.68	Joback Method
cpg	451.86	J/mol×K	612.28	Joback Method
cpg	468.76	J/mol×K	647.88	Joback Method
cpg	484.77	J/mol×K	683.48	Joback Method
cpg	499.99	J/mol×K	719.08	Joback Method
cpg	514.53	J/mol×K	754.67	Joback Method
cpg	528.49	J/mol×K	790.27	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=R216454&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume