

trans-2-Isopropyl-4-t-butylcyclohexanone

Inchi:	InChI=1S/C13H24O/c1-9(2)11-8-10(13(3,4)5)6-7-12(11)14/h9-11H,6-8H2,1-5H3/t10-,11-
InchiKey:	INDSELFLOGICC-GHMZBOCLSA-N
Formula:	C13H24O
SMILES:	CC(C)C1CC(C(C)(C)C)CCC1=O
Mol. weight [g/mol]:	196.33
CAS:	54513-98-3

Physical Properties

Property code	Value	Unit	Source
gf	-46.87	kJ/mol	Joback Method
hf	-429.40	kJ/mol	Joback Method
hfus	10.90	kJ/mol	Joback Method
hvap	47.22	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.674		Crippen Method
mcvol	184.740	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
tb	575.87	K	Joback Method
tc	796.38	K	Joback Method
tf	295.05	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.77	J/molxK	575.87	Joback Method
cpg	515.76	J/molxK	612.62	Joback Method
cpg	537.43	J/molxK	649.37	Joback Method
cpg	557.82	J/molxK	686.13	Joback Method
cpg	576.94	J/molxK	722.88	Joback Method
cpg	594.81	J/molxK	759.63	Joback Method
cpg	611.47	J/molxK	796.38	Joback Method

Sources

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=C54513983&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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