2,2,4,4-Tetramethyl-6-(3-methylbutanoyl)cyclohex

Other names: Leptospermone
1,3,5-Cyclohexanetrione, 2,2,4,4-tetramethyl-6-(3-methyl-1-oxobutyl)-
1,3,5-Cyclohexanetrione, 6-isovaleryl-2,2,4,4-tetramethyl-
Inchi: InChI=1S/C15H22O4/c1-8(2)7-9(16)10-11(17)14(3,4)13(19)15(5,6)12(10)18/h8,10H,7H2
InchiKey: YDWYMAHAWHBPPT-UHFFFAOYSA-N
Formula: C15H22O4
SMILES: CC(C)CC(=O)C1C(=O)C(C)(C)C(=O)C(C)(C)C1=O
Mol. weight [g/mol]: 266.33
CAS: 567-75-9

Physical Properties

Property code	Value	Unit	Source
gf	-425.66	kJ/mol	Joback Method
hf	-839.77	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	65.59	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.991		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1596.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	810.18	K	Joback Method
tc	1053.64	K	Joback Method
tf	545.10	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.91	J/mol×K	810.18	Joback Method

cpg	718.10	J/mol×K	850.76	Joback Method
cpg	738.83	J/mol×K	891.33	Joback Method
cpg	759.24	J/mol×K	931.91	Joback Method
cpg	779.49	J/mol×K	972.49	Joback Method
cpg	799.71	J/mol×K	1013.07	Joback Method
cpg	820.06	J/mol×K	1053.64	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=C567759&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