Hexanedioic acid, bis(1,3-dimethylbutyl) ester

Other names: Adipic acid, bis(1,3-dimethylbutyl) ester
di-(1,3-Dimethylbutyl)adipate
Adipic acid, di(4-methylpent-2-yl) ester
Inchi: InChI=1S/C18H34O4/c1-13(2)11-15(5)21-17(19)9-7-8-10-18(20)22-16(6)12-14(3)4/h13-1
InchiKey: LYHRWRRIMHVFFZ-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CC(C)CC(C)OC(=O)CCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 314.46
CAS: 55125-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-376.92	kJ/mol	Joback Method
hf	-925.57	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.502		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	1864.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	762.06	K	Joback Method
tc	946.82	K	Joback Method
tf	376.94	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.43	J/mol×K	762.06	Joback Method
cpg	869.48	J/mol×K	792.85	Joback Method
cpg	886.51	J/mol×K	823.65	Joback Method

cpg	902.54	J/mol×K	854.44	Joback Method
cpg	917.58	J/mol×K	885.24	Joback Method
cpg	931.65	J/mol×K	916.03	Joback Method
cpg	944.75	J/mol×K	946.82	Joback Method
dvisc	0.0024596	Pa×s	376.94	Joback Method
dvisc	0.0008051	Pa×s	441.13	Joback Method
dvisc	0.0003500	Pa×s	505.31	Joback Method
dvisc	0.0001836	Pa×s	569.50	Joback Method
dvisc	0.0001097	Pa×s	633.69	Joback Method
dvisc	0.0000721	Pa×s	697.87	Joback Method
dvisc	0.0000509	Pa×s	762.06	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=C55125229&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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