

Adipic acid, isobutyl 3-oxobut-2-yl ester

Inchi:	InChI=1S/C14H24O5/c1-10(2)9-18-13(16)7-5-6-8-14(17)19-12(4)11(3)15/h10,12H,5-9H2
InchiKey:	DNONBDMNPCQCCB-UHFFFAOYSA-N
Formula:	C14H24O5
SMILES:	CC(=O)C(C)OC(=O)CCCC(=O)OCC(C)C
Mol. weight [g/mol]:	272.34

Physical Properties

Property code	Value	Unit	Source
gf	-534.64	kJ/mol	Joback Method
hf	-945.03	kJ/mol	Joback Method
hfus	32.14	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.267		Crippen Method
mvol	224.570	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	1649.00		NIST Webbook
tb	725.29	K	Joback Method
tc	913.53	K	Joback Method
tf	411.79	K	Joback Method
vc	0.862	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.84	J/molxK	725.29	Joback Method
cpg	659.70	J/molxK	756.66	Joback Method
cpg	673.72	J/molxK	788.04	Joback Method
cpg	686.91	J/molxK	819.41	Joback Method
cpg	699.26	J/molxK	850.78	Joback Method
cpg	710.79	J/molxK	882.15	Joback Method
cpg	721.49	J/molxK	913.53	Joback Method
dvisc	0.0016806	Paxs	411.79	Joback Method
dvisc	0.0008061	Paxs	464.04	Joback Method

dvisc	0.0004486	Paxs	516.29	Joback Method
dvisc	0.0002781	Paxs	568.54	Joback Method
dvisc	0.0001868	Paxs	620.79	Joback Method
dvisc	0.0001335	Paxs	673.04	Joback Method
dvisc	0.0001001	Paxs	725.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U353747&Units=SI

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

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