

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

Inchi:	InChI=1S/C18H32O5/c1-4-5-6-7-8-11-14-22-17(20)12-9-10-13-18(21)23-16(3)15(2)19/h1
InchiKey:	DNYQMGPBUNRZQV-UHFFFAOYSA-N
Formula:	C18H32O5
SMILES:	CCCCCCCCOC(=O)CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	328.44

Physical Properties

Property code	Value	Unit	Source
gf	-498.52	kJ/mol	Joback Method
hf	-1022.31	kJ/mol	Joback Method
hfus	46.03	kJ/mol	Joback Method
hvap	80.33	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.971		Crippen Method
mcvol	280.930	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpola	2230.00		NIST Webbook
tb	817.25	K	Joback Method
tc	1006.29	K	Joback Method
tf	471.87	K	Joback Method
vc	1.091	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.85	J/molxK	817.25	Joback Method
cpg	889.00	J/molxK	848.76	Joback Method
cpg	904.13	J/molxK	880.26	Joback Method
cpg	918.25	J/molxK	911.77	Joback Method
cpg	931.39	J/molxK	943.28	Joback Method
cpg	943.54	J/molxK	974.78	Joback Method
cpg	954.72	J/molxK	1006.29	Joback Method
dvisc	0.0009340	Paxs	471.87	Joback Method
dvisc	0.0004651	Paxs	529.43	Joback Method

dvisc	0.0002655	Paxs	587.00	Joback Method
dvisc	0.0001676	Paxs	644.56	Joback Method
dvisc	0.0001140	Paxs	702.12	Joback Method
dvisc	0.0000823	Paxs	759.69	Joback Method
dvisc	0.0000621	Paxs	817.25	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=U353752&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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