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

Inchi: InChI=1S/C17H30O5/c1-4-5-6-7-10-13-21-16(19)11-8-9-12-17(20)22-15(3)14(2)18/h15H
InchiKey: AWMCHQPZEOUGAF-UHFFFAOYSA-N
Formula: C17H30O5
SMILES: CCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 314.42

Physical Properties

Property code	Value	Unit	Source
gf	-506.94	kJ/mol	Joback Method
hf	-1001.67	kJ/mol	Joback Method
hfus	43.44	kJ/mol	Joback Method
hvap	78.11	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.581		Crippen Method
mcvol	266.840	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	2131.00		NIST Webbook
tb	794.37	K	Joback Method
tc	981.67	K	Joback Method
tf	460.60	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.28	J/mol×K	794.37	Joback Method
cpg	830.08	J/mol×K	825.59	Joback Method
cpg	844.92	J/mol×K	856.80	Joback Method
cpg	858.81	J/mol×K	888.02	Joback Method
cpg	871.76	J/mol×K	919.24	Joback Method
cpg	883.78	J/mol×K	950.45	Joback Method
cpg	894.88	J/mol×K	981.67	Joback Method
dvisc	0.0010403	Pa×s	460.60	Joback Method
dvisc	0.0005239	Pa×s	516.23	Joback Method

dvisc	0.0003015	Pa×s	571.86	Joback Method
dvisc	0.0001914	Pa×s	627.49	Joback Method
dvisc	0.0001308	Pa×s	683.11	Joback Method
dvisc	0.0000947	Pa×s	738.74	Joback Method
dvisc	0.0000717	Pa×s	794.37	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=U353751&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