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

Inchi: InChI=1S/C27H50O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-31-26(29)21-18-19
InchiKey: HJIJBOUTKAGJFY-UHFFFAOYSA-N
Formula: C27H50O5
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 454.68

Physical Properties

Property code	Value	Unit	Source
gf	-422.74	kJ/mol	Joback Method
hf	-1208.07	kJ/mol	Joback Method
hfus	69.34	kJ/mol	Joback Method
hvap	100.37	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.482		Crippen Method
mcvol	407.740	ml/mol	McGowan Method
pc	751.85	kPa	Joback Method
rinpol	3133.00		NIST Webbook
tb	1023.17	K	Joback Method
tc	1268.74	K	Joback Method
tf	573.30	K	Joback Method
vc	1.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1429.11	J/mol×K	1023.17	Joback Method
cpg	1449.04	J/mol×K	1064.10	Joback Method
cpg	1466.90	J/mol×K	1105.03	Joback Method
cpg	1482.76	J/mol×K	1145.96	Joback Method
cpg	1496.70	J/mol×K	1186.89	Joback Method
cpg	1508.77	J/mol×K	1227.82	Joback Method
cpg	1519.06	J/mol×K	1268.74	Joback Method
dvisc	0.0003041	Pa×s	573.30	Joback Method
dvisc	0.0001392	Pa×s	648.28	Joback Method

dvisc	0.0000749	Pa×s	723.26	Joback Method
dvisc	0.0000453	Pa×s	798.23	Joback Method
dvisc	0.0000299	Pa×s	873.21	Joback Method
dvisc	0.0000210	Pa×s	948.19	Joback Method
dvisc	0.0000156	Pa×s	1023.17	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=U353761&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