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

Inchi: InChI=1S/C28H52O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-24-32-27(30)22-19
InchiKey: HJBJHVIWAVIHHY-UHFFFAOYSA-N
Formula: C28H52O5
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 468.71

Physical Properties

Property code	Value	Unit	Source
gf	-414.32	kJ/mol	Joback Method
hf	-1228.71	kJ/mol	Joback Method
hfus	71.93	kJ/mol	Joback Method
hvap	102.59	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.872		Crippen Method
mcvol	421.830	ml/mol	McGowan Method
pc	713.77	kPa	Joback Method
rinpol	3237.00		NIST Webbook
tb	1046.05	K	Joback Method
tc	1303.92	K	Joback Method
tf	584.57	K	Joback Method
vc	1.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1493.07	J/mol×K	1046.05	Joback Method
cpg	1513.56	J/mol×K	1089.03	Joback Method
cpg	1531.76	J/mol×K	1132.01	Joback Method
cpg	1547.75	J/mol×K	1174.98	Joback Method
cpg	1561.63	J/mol×K	1217.96	Joback Method
cpg	1573.48	J/mol×K	1260.94	Joback Method
cpg	1583.38	J/mol×K	1303.92	Joback Method
dvisc	0.0002649	Pa×s	584.57	Joback Method
dvisc	0.0001203	Pa×s	661.48	Joback Method

dvisc	0.0000644	Pa×s	738.40	Joback Method
dvisc	0.0000388	Pa×s	815.31	Joback Method
dvisc	0.0000255	Pa×s	892.22	Joback Method
dvisc	0.0000179	Pa×s	969.14	Joback Method
dvisc	0.0000133	Pa×s	1046.05	Joback Method

Sources

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=U353762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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