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

Inchi: InChI=1S/C26H48O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-30-25(28)20-17-18-21
InchiKey: KNAPXEGDSZSYDG-UHFFFAOYSA-N
Formula: C26H48O5
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 440.66

Physical Properties

Property code	Value	Unit	Source
gf	-431.16	kJ/mol	Joback Method
hf	-1187.43	kJ/mol	Joback Method
hfus	66.75	kJ/mol	Joback Method
hvap	98.14	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	7.092		Crippen Method
mcvol	393.650	ml/mol	McGowan Method
pc	793.05	kPa	Joback Method
rinpol	3032.00		NIST Webbook
rinpol	3032.00		NIST Webbook
tb	1000.29	K	Joback Method
tc	1235.03	K	Joback Method
tf	562.03	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1365.44	J/mol×K	1000.29	Joback Method
cpg	1384.85	J/mol×K	1039.41	Joback Method
cpg	1402.37	J/mol×K	1078.54	Joback Method
cpg	1418.08	J/mol×K	1117.66	Joback Method
cpg	1432.02	J/mol×K	1156.78	Joback Method
cpg	1444.26	J/mol×K	1195.90	Joback Method
cpg	1454.85	J/mol×K	1235.03	Joback Method
dvisc	0.0003483	Pa×s	562.03	Joback Method

dvisc	0.0001607	Pa×s	635.07	Joback Method
dvisc	0.0000870	Pa×s	708.12	Joback Method
dvisc	0.0000528	Pa×s	781.16	Joback Method
dvisc	0.0000349	Pa×s	854.20	Joback Method
dvisc	0.0000246	Pa×s	927.25	Joback Method
dvisc	0.0000183	Pa×s	1000.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U353760&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