Adipic acid, 3,3-dimethylbut-2-yl dodecyl ester

Inchi: InChI=1S/C24H46O4/c1-6-7-8-9-10-11-12-13-14-17-20-27-22(25)18-15-16-19-23(26)28-
InchiKey: RTZXUXIDDIXZCJ-UHFFFAOYSA-N
Formula: C24H46O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 398.62

Physical Properties

Property code	Value	Unit	Source
gf	-316.24	kJ/mol	Joback Method
hf	-1042.32	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	85.65	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.989		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	863.53	kPa	Joback Method
rinpol	2603.00		NIST Webbook
tb	897.43	K	Joback Method
tc	1098.73	K	Joback Method
tf	491.98	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.06	J/mol×K	897.43	Joback Method
cpg	1237.89	J/mol×K	930.98	Joback Method
cpg	1256.38	J/mol×K	964.53	Joback Method
cpg	1273.61	J/mol×K	998.08	Joback Method
cpg	1289.60	J/mol×K	1031.63	Joback Method
cpg	1304.43	J/mol×K	1065.18	Joback Method
cpg	1318.12	J/mol×K	1098.73	Joback Method
dvisc	0.0005616	Pa×s	491.98	Joback Method
dvisc	0.0002329	Pa×s	559.56	Joback Method

dvisc	0.0001168	Pa×s	627.13	Joback Method
dvisc	0.0000670	Pa×s	694.71	Joback Method
dvisc	0.0000424	Pa×s	762.28	Joback Method
dvisc	0.0000289	Pa×s	829.86	Joback Method
dvisc	0.0000209	Pa×s	897.43	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=U353677&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

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