Adipic acid, 2,4-dimethylpent-3-yl hexadecyl ester

Inchi: InChI=1S/C29H56O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-21-24-32-27(30)22-19-20-

InchiKey: RRZWOCPKTFODDS-UHFFFAOYSA-N

Formula: C29H56O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-281.86	kJ/mol	Joback Method
hf	-1147.33	kJ/mol	Joback Method
hfus	65.87	kJ/mol	Joback Method
hvap	97.30	kJ/mol	Joback Method
log10ws	-9.32		Crippen Method
logp	8.795		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	662.21	kPa	Joback Method
rinpol	3093.00		NIST Webbook
rinpol	3093.00		NIST Webbook
tb	1014.18	K	Joback Method
tc	1258.93	K	Joback Method
tf	515.91	K	Joback Method
vc	1.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1540.49	J/mol×K	1014.18	Joback Method
cpg	1632.38	J/mol×K	1218.13	Joback Method
cpg	1618.04	J/mol×K	1177.34	Joback Method
cpg	1601.76	J/mol×K	1136.55	Joback Method
cpg	1583.46	J/mol×K	1095.76	Joback Method
cpg	1563.07	J/mol×K	1054.97	Joback Method
cpg	1644.87	J/mol×K	1258.93	Joback Method
dvisc	0.0000101	Pa×s	1014.18	Joback Method

dvisc	0.0000142	Pa×s	931.14	Joback Method
dvisc	0.0000214	Pa×s	848.09	Joback Method
dvisc	0.0000353	Pa×s	765.05	Joback Method
dvisc	0.0000655	Pa×s	682.00	Joback Method
dvisc	0.0001445	Pa×s	598.96	Joback Method
dvisc	0.0004111	Pa×s	515.91	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=U353533&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