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

Inchi: InChI=1S/C30H58O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-33-28(31)23-20-

InchiKey: XQURFCPKZGKBDJ-UHFFFAOYSA-N

Formula: C30H58O4

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

Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	-273.44	kJ/mol	Joback Method
hf	-1167.97	kJ/mol	Joback Method
hfus	68.46	kJ/mol	Joback Method
hvap	99.52	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	9.185		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	630.66	kPa	Joback Method
rinpol	3194.00		NIST Webbook
rinpol	3194.00		NIST Webbook
tb	1037.06	K	Joback Method
tc	1294.33	K	Joback Method
tf	527.18	K	Joback Method
vc	1.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1605.81	J/mol×K	1037.06	Joback Method
cpg	1698.82	J/mol×K	1251.45	Joback Method
cpg	1684.64	J/mol×K	1208.58	Joback Method
cpg	1668.35	J/mol×K	1165.70	Joback Method
cpg	1649.85	J/mol×K	1122.82	Joback Method
cpg	1629.04	J/mol×K	1079.94	Joback Method
cpg	1711.00	J/mol×K	1294.33	Joback Method
dvisc	0.0000086	Pa×s	1037.06	Joback Method

dvisc	0.0000121	Pa×s	952.08	Joback Method
dvisc	0.0000182	Pa×s	867.10	Joback Method
dvisc	0.0000300	Pa×s	782.12	Joback Method
dvisc	0.0000559	Pa×s	697.14	Joback Method
dvisc	0.0001236	Pa×s	612.16	Joback Method
dvisc	0.0003531	Pa×s	527.18	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=U353534&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