Adipic acid, heptadecyl 3-methylpentyl ester

Inchi: InChI=1S/C29H56O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-21-25-32-28(30)22-19-2
InchiKey: XDAXPJNIKKDDSL-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCC(C)CC
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-276.98	kJ/mol	Joback Method
hf	-1136.77	kJ/mol	Joback Method
hfus	72.92	kJ/mol	Joback Method
hvap	98.07	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.941		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	656.79	kPa	Joback Method
rinpol	3208.00		NIST Webbook
rinpol	3208.00		NIST Webbook
tb	1015.06	K	Joback Method
tc	1265.21	K	Joback Method
tf	545.91	K	Joback Method
vc	1.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.99	J/mol×K	1015.06	Joback Method
cpg	1563.19	J/mol×K	1056.75	Joback Method
cpg	1584.14	J/mol×K	1098.44	Joback Method
cpg	1602.93	J/mol×K	1140.13	Joback Method
cpg	1619.67	J/mol×K	1181.83	Joback Method
cpg	1634.42	J/mol×K	1223.52	Joback Method
cpg	1647.29	J/mol×K	1265.21	Joback Method
dvisc	0.0003091	Pa×s	545.91	Joback Method

dvisc	0.0001288	Pa×s	624.10	Joback Method
dvisc	0.0000652	Pa×s	702.29	Joback Method
dvisc	0.0000378	Pa×s	780.49	Joback Method
dvisc	0.0000242	Pa×s	858.68	Joback Method
dvisc	0.0000167	Pa×s	936.87	Joback Method
dvisc	0.0000122	Pa×s	1015.06	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=U353702&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