Adipic acid, octadecyl trans-hex-3-enyl ester

Inchi: InChI=1S/C30H56O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-24-28-34-30(32)26-
InchiKey: LHRFQEABUFKQIE-SOFGYWHQSA-N
Formula: C30H56O4
SMILES: CCC=CCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-185.90	kJ/mol	Joback Method
hf	-1034.91	kJ/mol	Joback Method
hfus	79.23	kJ/mol	Joback Method
hvap	100.64	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	9.251		Crippen Method
mcvol	444.140	ml/mol	McGowan Method
pc	639.63	kPa	Joback Method
rinpol	3345.00		NIST Webbook
rinpol	3345.00		NIST Webbook
tb	1042.54	K	Joback Method
tc	1305.36	K	Joback Method
tf	567.10	K	Joback Method
vc	1.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1576.88	J/mol×K	1042.54	Joback Method
cpg	1675.65	J/mol×K	1261.55	Joback Method
cpg	1659.71	J/mol×K	1217.75	Joback Method
cpg	1642.00	J/mol×K	1173.95	Joback Method
cpg	1622.38	J/mol×K	1130.15	Joback Method
cpg	1600.72	J/mol×K	1086.34	Joback Method
cpg	1689.94	J/mol×K	1305.36	Joback Method
dvisc	0.0000101	Pa×s	1042.54	Joback Method

dvisc	0.0000136	Pa×s	963.30	Joback Method
dvisc	0.0000195	Pa×s	884.06	Joback Method
dvisc	0.0000300	Pa×s	804.82	Joback Method
dvisc	0.0000505	Pa×s	725.58	Joback Method
dvisc	0.0000968	Pa×s	646.34	Joback Method
dvisc	0.0002224	Pa×s	567.10	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=U354022&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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