

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
mvol	444.140	ml/mol	McGowan Method
pc	639.63	kPa	Joback Method
rinpol	3345.00		NIST Webbook
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tb	1042.54	K	Joback Method
tc	1305.36	K	Joback Method
tf	567.10	K	Joback Method
vc	1.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1576.88	J/molxK	1042.54	Joback Method
cpg	1600.72	J/molxK	1086.34	Joback Method
cpg	1622.38	J/molxK	1130.15	Joback Method
cpg	1642.00	J/molxK	1173.95	Joback Method
cpg	1659.71	J/molxK	1217.75	Joback Method
cpg	1675.65	J/molxK	1261.55	Joback Method
cpg	1689.94	J/molxK	1305.36	Joback Method
dvisc	0.0002224	Paxs	567.10	Joback Method

dvisc	0.0000968	Paxs	646.34	Joback Method
dvisc	0.0000505	Paxs	725.58	Joback Method
dvisc	0.0000300	Paxs	804.82	Joback Method
dvisc	0.0000195	Paxs	884.06	Joback Method
dvisc	0.0000136	Paxs	963.30	Joback Method
dvisc	0.0000101	Paxs	1042.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354022&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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