

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

Inchi:	InChI=1S/C15H26O4/c1-3-5-6-9-13-19-15(17)11-8-7-10-14(16)18-12-4-2/h5-6H,3-4,7-13
InchiKey:	LDUPTVVUACLBMO-AATRIKPKSA-N
Formula:	C15H26O4
SMILES:	CCC=CCCOC(=O)CCCCC(=O)OCCC
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-312.20	kJ/mol	Joback Method
hf	-725.31	kJ/mol	Joback Method
hfus	40.38	kJ/mol	Joback Method
hvap	67.25	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.399		Crippen Method
mvol	232.790	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	1852.00		NIST Webbook
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tb	699.34	K	Joback Method
tc	880.04	K	Joback Method
tf	398.05	K	Joback Method
vc	0.903	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.66	J/molxK	699.34	Joback Method
cpg	670.28	J/molxK	729.46	Joback Method
cpg	685.13	J/molxK	759.57	Joback Method
cpg	699.22	J/molxK	789.69	Joback Method
cpg	712.57	J/molxK	819.81	Joback Method
cpg	725.18	J/molxK	849.93	Joback Method
cpg	737.08	J/molxK	880.04	Joback Method
dvisc	0.0012706	Paxs	398.05	Joback Method

dvisc	0.0006402	Paxs	448.26	Joback Method
dvisc	0.0003703	Paxs	498.48	Joback Method
dvisc	0.0002368	Paxs	548.69	Joback Method
dvisc	0.0001632	Paxs	598.91	Joback Method
dvisc	0.0001192	Paxs	649.12	Joback Method
dvisc	0.0000910	Paxs	699.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354006&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

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