

Adipic acid, cis-non-3-enyl tridecyl ester

Inchi:	InChI=1S/C28H52O4/c1-3-5-7-9-11-12-13-14-16-18-22-26-32-28(30)24-20-19-23-27(29)
InchiKey:	HRTWPARABUCIRA-ICFOKQHNSA-N
Formula:	C28H52O4
SMILES:	CCCCC=CCCOC(=O)CCCC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]:	452.71

Physical Properties

Property code	Value	Unit	Source
gf	-202.74	kJ/mol	Joback Method
hf	-993.63	kJ/mol	Joback Method
hfus	74.05	kJ/mol	Joback Method
hvap	96.19	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.471		Crippen Method
mvol	415.960	ml/mol	McGowan Method
pc	706.58	kPa	Joback Method
rinpol	3124.00		NIST Webbook
rinpol	3124.00		NIST Webbook
tb	996.78	K	Joback Method
tc	1234.53	K	Joback Method
tf	544.56	K	Joback Method
vc	1.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.46	J/molxK	996.78	Joback Method
cpg	1468.63	J/molxK	1036.40	Joback Method
cpg	1489.00	J/molxK	1076.03	Joback Method
cpg	1507.66	J/molxK	1115.65	Joback Method
cpg	1524.71	J/molxK	1155.28	Joback Method
cpg	1540.23	J/molxK	1194.90	Joback Method
cpg	1554.32	J/molxK	1234.53	Joback Method
dvisc	0.0002922	Paxs	544.56	Joback Method

dvisc	0.0001291	Paxs	619.93	Joback Method
dvisc	0.0000681	Paxs	695.30	Joback Method
dvisc	0.0000407	Paxs	770.67	Joback Method
dvisc	0.0000266	Paxs	846.04	Joback Method
dvisc	0.0000187	Paxs	921.41	Joback Method
dvisc	0.0000139	Paxs	996.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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