

Phthalic acid, cis-hex-3-enyl pentadecyl ester

Inchi:	InChI=1S/C29H46O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-21-25-33-29(31)27-23-19-18-
InchiKey:	MXMVDZVYKLRZRW-VURMDHGXSA-N
Formula:	C29H46O4
SMILES:	CCC=CCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	458.67

Physical Properties

Property code	Value	Unit	Source
gf	-91.54	kJ/mol	Joback Method
hf	-789.21	kJ/mol	Joback Method
hfus	70.29	kJ/mol	Joback Method
hvap	101.36	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.448		Crippen Method
mvol	406.290	ml/mol	McGowan Method
pc	797.08	kPa	Joback Method
rinpol	3254.00		NIST Webbook
rinpol	3254.00		NIST Webbook
tb	1051.32	K	Joback Method
tc	1293.56	K	Joback Method
tf	594.77	K	Joback Method
vc	1.579	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1404.37	J/molxK	1051.32	Joback Method
cpg	1481.02	J/molxK	1253.18	Joback Method
cpg	1468.62	J/molxK	1212.81	Joback Method
cpg	1454.85	J/molxK	1172.44	Joback Method
cpg	1439.62	J/molxK	1132.07	Joback Method
cpg	1422.82	J/molxK	1091.69	Joback Method
cpg	1492.17	J/molxK	1293.56	Joback Method
dvisc	0.0000126	Paxs	1051.32	Joback Method

dvisc	0.0000166	Paxs	975.23	Joback Method
dvisc	0.0000230	Paxs	899.14	Joback Method
dvisc	0.0000338	Paxs	823.04	Joback Method
dvisc	0.0000537	Paxs	746.95	Joback Method
dvisc	0.0000946	Paxs	670.86	Joback Method
dvisc	0.0001929	Paxs	594.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360392&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

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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