

Phthalic acid, tetradecyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C28H44O4/c1-3-5-7-9-10-11-12-13-14-15-16-20-24-32-28(30)26-22-18-17-21-
InchiKey:	BAODKCCXUCGTKT-SOFGYWHQSA-N
Formula:	C28H44O4
SMILES:	CCC=CCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]:	444.65

Physical Properties

Property code	Value	Unit	Source
gf	-99.96	kJ/mol	Joback Method
hf	-768.57	kJ/mol	Joback Method
hfus	67.70	kJ/mol	Joback Method
hvap	99.13	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.058		Crippen Method
mcvol	392.200	ml/mol	McGowan Method
pc	842.11	kPa	Joback Method
rinpol	3144.00		NIST Webbook
tb	1028.44	K	Joback Method
tc	1262.21	K	Joback Method
tf	583.50	K	Joback Method
vc	1.524	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1340.94	J/mol×K	1028.44	Joback Method
cpg	1358.94	J/mol×K	1067.40	Joback Method
cpg	1375.39	J/mol×K	1106.36	Joback Method
cpg	1390.37	J/mol×K	1145.33	Joback Method
cpg	1403.97	J/mol×K	1184.29	Joback Method
cpg	1416.27	J/mol×K	1223.25	Joback Method
cpg	1427.36	J/mol×K	1262.21	Joback Method
dvisc	0.0002193	Paxs	583.50	Joback Method
dvisc	0.0001085	Paxs	657.66	Joback Method

dvisc	0.0000619	Paxs	731.81	Joback Method
dvisc	0.0000392	Paxs	805.97	Joback Method
dvisc	0.0000268	Paxs	880.13	Joback Method
dvisc	0.0000194	Paxs	954.28	Joback Method
dvisc	0.0000147	Paxs	1028.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360492&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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