

Terephthalic acid, but-3-enyl hexadecyl ester

Inchi:	InChI=1S/C28H44O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-24-32-28(30)26-21-19-2
InchiKey:	XCVVRVDBEWZCDT-UHFFFAOYSA-N
Formula:	C28H44O4
SMILES:	C=CCCOC(=O)c1ccc(C(=O)OCCCCCCCCCCCCCCCCC)cc1
Mol. weight [g/mol]:	444.65

Physical Properties

Property code	Value	Unit	Source
gf	-92.34	kJ/mol	Joback Method
hf	-760.36	kJ/mol	Joback Method
hfus	66.22	kJ/mol	Joback Method
hvap	98.50	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.058		Crippen Method
mvol	392.200	ml/mol	McGowan Method
pc	837.24	kPa	Joback Method
rinpol	3397.00		NIST Webbook
tb	1020.96	K	Joback Method
tc	1253.49	K	Joback Method
tf	586.82	K	Joback Method
vc	1.524	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1339.18	J/molxK	1020.96	Joback Method
cpg	1356.99	J/molxK	1059.72	Joback Method
cpg	1373.13	J/molxK	1098.47	Joback Method
cpg	1387.69	J/molxK	1137.23	Joback Method
cpg	1400.74	J/molxK	1175.98	Joback Method
cpg	1412.36	J/molxK	1214.74	Joback Method
cpg	1422.61	J/molxK	1253.49	Joback Method
dvisc	0.0002465	Paxs	586.82	Joback Method
dvisc	0.0001257	Paxs	659.18	Joback Method

dvisc	0.0000732	Paxs	731.53	Joback Method
dvisc	0.0000470	Paxs	803.89	Joback Method
dvisc	0.0000325	Paxs	876.25	Joback Method
dvisc	0.0000237	Paxs	948.60	Joback Method
dvisc	0.0000181	Paxs	1020.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356346&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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