Phthalic acid, 8-chlorooctyl dodecyl ester

Inchi: InChI=1S/C28H45ClO4/c1-2-3-4-5-6-7-8-10-13-18-23-32-27(30)25-20-15-16-21-26(25)28

InchiKey: HNLXZGCHJULIFA-UHFFFAOYSA-N

Formula: C28H45ClO4

SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 481.11

Physical Properties

Property code	Value	Unit	Source
gf	-192.11	kJ/mol	Joback Method
hf	-901.53	kJ/mol	Joback Method
hfus	71.70	kJ/mol	Joback Method
hvap	103.56	kJ/mol	Joback Method
log10ws	-9.64		Crippen Method
logp	8.500		Crippen Method
mcvol	408.740	ml/mol	McGowan Method
pc	800.24	kPa	Joback Method
rinpol	3471.00		NIST Webbook
rinpol	3471.00		NIST Webbook
tb	1061.71	K	Joback Method
tc	1308.18	K	Joback Method
tf	618.50	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.96	J/mol×K	1061.71	Joback Method
cpg	1412.04	J/mol×K	1102.79	Joback Method
cpg	1427.27	J/mol×K	1143.87	Joback Method
cpg	1440.73	J/mol×K	1184.94	Joback Method
cpg	1452.50	J/mol×K	1226.02	Joback Method
cpg	1462.66	J/mol×K	1267.10	Joback Method
cpg	1471.32	J/mol×K	1308.18	Joback Method
dvisc	0.0001855	Pa×s	618.50	Joback Method

dvisc	0.0000957	Pa×s	692.37	Joback Method
dvisc	0.0000561	Pa×s	766.24	Joback Method
dvisc	0.0000361	Pa×s	840.11	Joback Method
dvisc	0.0000250	Pa×s	913.97	Joback Method
dvisc	0.0000182	Pa×s	987.84	Joback Method
dvisc	0.0000139	Pa×s	1061.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U356867&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