Terephthalic acid, 4-chloro-2-methylbenzyl octyl ester

Inchi: InChI=1S/C24H29ClO4/c1-3-4-5-6-7-8-15-28-23(26)19-9-11-20(12-10-19)24(27)29-17-21

InchiKey: PWLGSHWEKRDQEW-UHFFFAOYSA-N

Formula: C24H29ClO4

SMILES: CCCCCCCCOC(=O)c1ccc(C(=O)OCc2ccc(Cl)cc2C)cc1

Mol. weight [g/mol]: 416.94

Physical Properties

Property code	Value	Unit	Source
gf	-132.64	kJ/mol	Joback Method
hf	-605.38	kJ/mol	Joback Method
hfus	54.60	kJ/mol	Joback Method
hvap	98.25	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	6.523		Crippen Method
mcvol	328.620	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2728.00		NIST Webbook
rinpol	2728.00		NIST Webbook
tb	1006.83	K	Joback Method
tc	1237.08	K	Joback Method
tf	624.88	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.08	J/mol×K	1006.83	Joback Method
cpg	1049.89	J/mol×K	1045.20	Joback Method
cpg	1061.25	J/mol×K	1083.58	Joback Method
cpg	1071.22	J/mol×K	1121.95	Joback Method
cpg	1079.83	J/mol×K	1160.33	Joback Method
cpg	1087.13	J/mol×K	1198.70	Joback Method
cpg	1093.16	J/mol×K	1237.08	Joback Method
dvisc	0.0002222	Pa×s	624.88	Joback Method

dvisc	0.0001345	Pa×s	688.54	Joback Method
dvisc	0.0000887	Pa×s	752.20	Joback Method
dvisc	0.0000624	Pa×s	815.86	Joback Method
dvisc	0.0000462	Pa×s	879.51	Joback Method
dvisc	0.0000356	Pa×s	943.17	Joback Method
dvisc	0.0000284	Pa×s	1006.83	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=U416113&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