Terephthalic acid, 2-chloropropyl tetradecyl ester

Inchi: InChI=1S/C25H39ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-19-29-24(27)22-15-17-23(18-16

InchiKey: ICZTVBPGIRXLPB-UHFFFAOYSA-N

Formula: C25H39ClO4

SMILES: CCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(C)Cl)cc1

Mol. weight [g/mol]: 439.03

Physical Properties

Property code	Value	Unit	Source
gf	-219.81	kJ/mol	Joback Method
hf	-844.89	kJ/mol	Joback Method
hfus	60.41	kJ/mol	Joback Method
hvap	96.49	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	7.329		Crippen Method
mcvol	366.470	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	3195.00		NIST Webbook
rinpol	3195.00		NIST Webbook
tb	992.63	K	Joback Method
tc	1215.36	K	Joback Method
tf	569.69	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1208.08	J/mol×K	992.63	Joback Method
cpg	1224.12	J/mol×K	1029.75	Joback Method
cpg	1238.67	J/mol×K	1066.87	Joback Method
cpg	1251.76	J/mol×K	1103.99	Joback Method
cpg	1263.44	J/mol×K	1141.12	Joback Method
cpg	1273.77	J/mol×K	1178.24	Joback Method
cpg	1282.81	J/mol×K	1215.36	Joback Method
dvisc	0.0002979	Pa×s	569.69	Joback Method

dvisc	0.0001488	Pa×s	640.18	Joback Method
dvisc	0.0000853	Pa×s	710.67	Joback Method
dvisc	0.0000540	Pa×s	781.16	Joback Method
dvisc	0.0000369	Pa×s	851.65	Joback Method
dvisc	0.0000268	Pa×s	922.14	Joback Method
dvisc	0.0000203	Pa×s	992.63	Joback Method

Sources

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=U356179&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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