Terephthalic acid, 2-chloropropyl decyl ester

Inchi: InChI=1S/C21H31ClO4/c1-3-4-5-6-7-8-9-10-15-25-20(23)18-11-13-19(14-12-18)21(24)26
InchiKey: AUHPJSKSQHHXHG-UHFFFAOYSA-N
Formula: C21H31ClO4
SMILES: CCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(C)Cl)cc1
Mol. weight [g/mol]: 382.92

Physical Properties

Property code	Value	Unit	Source
gf	-253.49	kJ/mol	Joback Method
hf	-762.33	kJ/mol	Joback Method
hfus	50.05	kJ/mol	Joback Method
hvap	87.59	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.768		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	901.11	K	Joback Method
tc	1109.38	K	Joback Method
tf	524.61	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.82	J/mol×K	901.11	Joback Method
cpg	1029.03	J/mol×K	1074.67	Joback Method
cpg	1018.52	J/mol×K	1039.96	Joback Method
cpg	1006.88	J/mol×K	1005.25	Joback Method
cpg	994.07	J/mol×K	970.53	Joback Method
cpg	980.06	J/mol×K	935.82	Joback Method
cpg	1038.42	J/mol×K	1109.38	Joback Method
dvisc	0.0000373	Pa×s	901.11	Joback Method

dvisc	0.0000487	Pa×s	838.36	Joback Method
dvisc	0.0000664	Pa×s	775.61	Joback Method
dvisc	0.0000957	Pa×s	712.86	Joback Method
dvisc	0.0001479	Pa×s	650.11	Joback Method
dvisc	0.0002509	Pa×s	587.36	Joback Method
dvisc	0.0004830	Pa×s	524.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356177&Units=SI
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

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