Terephthalic acid, 2-chloropropyl ethyl ester

Inchi: InChI=1S/C13H15ClO4/c1-3-17-12(15)10-4-6-11(7-5-10)13(16)18-8-9(2)14/h4-7,9H,3,8H
InchiKey: JSRPCJSBWSJEIY-UHFFFAOYSA-N
Formula: C13H15ClO4
SMILES: CCOC(=O)c1ccc(C(=O)OCC(C)Cl)cc1
Mol. weight [g/mol]: 270.71

Physical Properties

Property code	Value	Unit	Source
gf	-320.85	kJ/mol	Joback Method
hf	-597.21	kJ/mol	Joback Method
hfus	29.33	kJ/mol	Joback Method
hvap	69.78	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.647		Crippen Method
mcvol	197.390	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	1951.00		NIST Webbook
tb	718.07	K	Joback Method
tc	933.75	K	Joback Method
tf	434.45	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.64	J/mol×K	718.07	Joback Method
cpg	526.77	J/mol×K	754.02	Joback Method
cpg	538.97	J/mol×K	789.96	Joback Method
cpg	550.27	J/mol×K	825.91	Joback Method
cpg	560.66	J/mol×K	861.85	Joback Method
cpg	570.15	J/mol×K	897.80	Joback Method
cpg	578.75	J/mol×K	933.75	Joback Method
dvisc	0.0010572	Pa×s	434.45	Joback Method
dvisc	0.0006062	Pa×s	481.72	Joback Method

dvisc	0.0003839	Pa×s	528.99	Joback Method
dvisc	0.0002621	Pa×s	576.26	Joback Method
dvisc	0.0001896	Pa×s	623.53	Joback Method
dvisc	0.0001435	Pa×s	670.80	Joback Method
dvisc	0.0001127	Pa×s	718.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356167&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