

Terephthalic acid, 2-chloropropyl isoheptyl ester

Inchi:	InChI=1S/C17H23ClO4/c1-12(2)5-4-10-21-16(19)14-6-8-15(9-7-14)17(20)22-11-13(3)18
InchiKey:	HVDWJPLMXLZPFX-UHFFFAOYSA-N
Formula:	C17H23ClO4
SMILES:	CC(C)CCCOC(=O)c1ccc(C(=O)OCC(C)Cl)cc1
Mol. weight [g/mol]:	326.81

Physical Properties

Property code	Value	Unit	Source
gf	-289.61	kJ/mol	Joback Method
hf	-685.05	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	78.30	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.064		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinsol	2331.00		NIST Webbook
tb	809.15	K	Joback Method
tc	1018.80	K	Joback Method
tf	464.53	K	Joback Method
vc	0.965	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.45	J/molxK	809.15	Joback Method
cpg	747.08	J/molxK	844.09	Joback Method
cpg	760.60	J/molxK	879.03	Joback Method
cpg	773.05	J/molxK	913.98	Joback Method
cpg	784.43	J/molxK	948.92	Joback Method
cpg	794.77	J/molxK	983.86	Joback Method
cpg	804.08	J/molxK	1018.80	Joback Method
dvisc	0.0008514	Paxs	464.53	Joback Method
dvisc	0.0004307	Paxs	521.97	Joback Method

dvisc	0.0002494	Paxs	579.40	Joback Method
dvisc	0.0001594	Paxs	636.84	Joback Method
dvisc	0.0001097	Paxs	694.28	Joback Method
dvisc	0.0000799	Paxs	751.71	Joback Method
dvisc	0.0000609	Paxs	809.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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