

Phthalic acid, 2-(3-chlorophenyl)ethyl heptyl ester

Inchi:	InChI=1S/C23H27ClO4/c1-2-3-4-5-8-15-27-22(25)20-12-6-7-13-21(20)23(26)28-16-14-18
InchiKey:	ONPXCGQAEXMJMM-UHFFFAOYSA-N
Formula:	C23H27ClO4
SMILES:	CCCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Cl)c1
Mol. weight [g/mol]:	402.91

Physical Properties

Property code	Value	Unit	Source
gf	-131.43	kJ/mol	Joback Method
hf	-573.27	kJ/mol	Joback Method
hfus	52.40	kJ/mol	Joback Method
hvap	95.37	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	5.867		Crippen Method
mcvol	314.530	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	3005.00		NIST Webbook
tb	978.97	K	Joback Method
tc	1206.69	K	Joback Method
tf	601.09	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.77	J/molxK	978.97	Joback Method
cpg	991.68	J/molxK	1016.92	Joback Method
cpg	1003.22	J/molxK	1054.88	Joback Method
cpg	1013.44	J/molxK	1092.83	Joback Method
cpg	1022.39	J/molxK	1130.78	Joback Method
cpg	1030.12	J/molxK	1168.74	Joback Method
cpg	1036.67	J/molxK	1206.69	Joback Method
dvisc	0.0002752	Paxs	601.09	Joback Method
dvisc	0.0001623	Paxs	664.07	Joback Method

dvisc	0.0001049	Paxs	727.05	Joback Method
dvisc	0.0000726	Paxs	790.03	Joback Method
dvisc	0.0000531	Paxs	853.01	Joback Method
dvisc	0.0000406	Paxs	915.99	Joback Method
dvisc	0.0000321	Paxs	978.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377857&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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