

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

Inchi:	InChI=1S/C24H20Cl2O4/c25-19-7-3-5-17(15-19)11-13-29-23(27)21-9-1-2-10-22(21)24(2
InchiKey:	KHNJKNHMRGYYOX-UHFFFAOYSA-N
Formula:	C24H20Cl2O4
SMILES:	O=C(OCCc1cccc(Cl)c1)c1cccc1C(=O)OCCc1cccc(Cl)c1
Mol. weight [g/mol]:	443.32

Physical Properties

Property code	Value	Unit	Source
gf	-32.16	kJ/mol	Joback Method
hf	-384.59	kJ/mol	Joback Method
hfus	52.84	kJ/mol	Joback Method
hvap	104.91	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	5.792		Crippen Method
mcvol	317.100	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	3200.00		NIST Webbook
tb	1070.94	K	Joback Method
tc	1324.89	K	Joback Method
tf	681.22	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.59	J/molxK	1070.94	Joback Method
cpg	951.40	J/molxK	1113.26	Joback Method
cpg	958.79	J/molxK	1155.59	Joback Method
cpg	964.82	J/molxK	1197.91	Joback Method
cpg	969.57	J/molxK	1240.24	Joback Method
cpg	973.11	J/molxK	1282.56	Joback Method
cpg	975.53	J/molxK	1324.89	Joback Method
dvisc	0.0001705	Paxs	681.22	Joback Method
dvisc	0.0001077	Paxs	746.17	Joback Method

dvisc	0.0000732	Paxs	811.13	Joback Method
dvisc	0.0000527	Paxs	876.08	Joback Method
dvisc	0.0000397	Paxs	941.03	Joback Method
dvisc	0.0000310	Paxs	1005.99	Joback Method
dvisc	0.0000250	Paxs	1070.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377865&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

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