

Isophthalic acid, 2,5-dichlorophenyl hexyl ester

Inchi:

InChI=1S/C20H20Cl2O4/c1-2-3-4-5-11-25-19(23)14-7-6-8-15(12-14)20(24)26-18-13-16(2)

InchiKey:

ZRBGPBQTLYIPDA-UHFFFAOYSA-N

Formula:

C20H20Cl2O4

SMILES:

CCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)ccc2Cl)c1

Mol. weight [g/mol]:

395.28

Physical Properties

Property code	Value	Unit	Source
gf	-178.25	kJ/mol	Joback Method
hf	-538.56	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	93.73	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	5.950		Crippen Method
mcvol	284.500	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	3008.00		NIST Webbook
rinpol	3008.00		NIST Webbook
tb	952.74	K	Joback Method
tc	1185.41	K	Joback Method
tf	609.72	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.06	J/molxK	952.74	Joback Method
cpg	866.57	J/molxK	1146.64	Joback Method
cpg	860.32	J/molxK	1107.86	Joback Method
cpg	852.87	J/molxK	1069.08	Joback Method
cpg	844.20	J/molxK	1030.30	Joback Method
cpg	834.27	J/molxK	991.52	Joback Method
cpg	871.66	J/molxK	1185.41	Joback Method
dvisc	0.0000433	Paxs	952.74	Joback Method

dvisc	0.0000537	Paxs	895.57	Joback Method
dvisc	0.0000684	Paxs	838.40	Joback Method
dvisc	0.0000903	Paxs	781.23	Joback Method
dvisc	0.0001246	Paxs	724.06	Joback Method
dvisc	0.0001817	Paxs	666.89	Joback Method
dvisc	0.0002844	Paxs	609.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344702&Units=SI

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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