

Isophthalic acid, 3,5-dichlorophenyl heptyl ester

Inchi:	InChI=1S/C21H22Cl2O4/c1-2-3-4-5-6-10-26-20(24)15-8-7-9-16(11-15)21(25)27-19-13-17
InchiKey:	GKMGNDKPFMDPIP-UHFFFAOYSA-N
Formula:	C21H22Cl2O4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)cc(Cl)c2)c1
Mol. weight [g/mol]:	409.30

Physical Properties

Property code	Value	Unit	Source
gf	-169.83	kJ/mol	Joback Method
hf	-559.20	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	95.96	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.340		Crippen Method
mcvol	298.590	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinsol	3032.00		NIST Webbook
tb	975.62	K	Joback Method
tc	1207.92	K	Joback Method
tf	620.99	K	Joback Method
vc	1.141	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.88	J/molxK	975.62	Joback Method
cpg	892.17	J/molxK	1014.34	Joback Method
cpg	902.14	J/molxK	1053.05	Joback Method
cpg	910.83	J/molxK	1091.77	Joback Method
cpg	918.26	J/molxK	1130.49	Joback Method
cpg	924.49	J/molxK	1169.20	Joback Method
cpg	929.54	J/molxK	1207.92	Joback Method
dvisc	0.0002554	Paxs	620.99	Joback Method
dvisc	0.0001614	Paxs	680.10	Joback Method

dvisc	0.0001098	Paxs	739.20	Joback Method
dvisc	0.0000790	Paxs	798.30	Joback Method
dvisc	0.0000595	Paxs	857.41	Joback Method
dvisc	0.0000465	Paxs	916.51	Joback Method
dvisc	0.0000375	Paxs	975.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356586&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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