

Isophthalic acid, 3-chlorophenyl heptyl ester

Inchi:	InChI=1S/C21H23ClO4/c1-2-3-4-5-6-13-25-20(23)16-9-7-10-17(14-16)21(24)26-19-12-8
InchiKey:	XALCYISEOJIBTB-UHFFFAOYSA-N
Formula:	C21H23ClO4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)Oc2cccc(Cl)c2)c1
Mol. weight [g/mol]:	374.86

Physical Properties

Property code	Value	Unit	Source
gf	-148.27	kJ/mol	Joback Method
hf	-531.99	kJ/mol	Joback Method
hfus	47.22	kJ/mol	Joback Method
hvap	90.91	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	5.686		Crippen Method
mcvol	286.350	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2982.00		NIST Webbook
tb	933.21	K	Joback Method
tc	1160.36	K	Joback Method
tf	578.55	K	Joback Method
vc	1.093	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.25	J/molxK	933.21	Joback Method
cpg	874.03	J/molxK	971.07	Joback Method
cpg	885.51	J/molxK	1008.93	Joback Method
cpg	895.72	J/molxK	1046.79	Joback Method
cpg	904.71	J/molxK	1084.65	Joback Method
cpg	912.52	J/molxK	1122.50	Joback Method
cpg	919.18	J/molxK	1160.36	Joback Method
dvisc	0.0003421	Paxs	578.55	Joback Method
dvisc	0.0002062	Paxs	637.66	Joback Method

dvisc	0.0001354	Paxs	696.77	Joback Method
dvisc	0.0000950	Paxs	755.88	Joback Method
dvisc	0.0000701	Paxs	814.99	Joback Method
dvisc	0.0000540	Paxs	874.10	Joback Method
dvisc	0.0000429	Paxs	933.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344606&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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