

Isophthalic acid, 3-chlorophenyl isoheptyl ester

Inchi: InChI=1S/C20H21ClO4/c1-14(2)6-5-11-24-19(22)15-7-3-8-16(12-15)20(23)25-18-10-4-9
InchiKey: RMJBZOJHCKOGOE-UHFFFAOYSA-N
Formula: C20H21ClO4
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2cccc(Cl)c2)c1
Mol. weight [g/mol]: 360.83

Physical Properties

Property code	Value	Unit	Source
gf	-159.13	kJ/mol	Joback Method
hf	-516.63	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	88.30	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.152		Crippen Method
mvol	272.260	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2816.00		NIST Webbook
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tb	909.89	K	Joback Method
tc	1140.67	K	Joback Method
tf	552.28	K	Joback Method
vc	1.030	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.93	J/molxK	909.89	Joback Method
cpg	816.74	J/molxK	948.35	Joback Method
cpg	828.22	J/molxK	986.82	Joback Method
cpg	838.42	J/molxK	1025.28	Joback Method
cpg	847.38	J/molxK	1063.74	Joback Method
cpg	855.12	J/molxK	1102.21	Joback Method
cpg	861.68	J/molxK	1140.67	Joback Method
dvisc	0.0004114	Paxs	552.28	Joback Method

dvisc	0.0002380	Paxs	611.88	Joback Method
dvisc	0.0001517	Paxs	671.48	Joback Method
dvisc	0.0001041	Paxs	731.09	Joback Method
dvisc	0.0000756	Paxs	790.69	Joback Method
dvisc	0.0000574	Paxs	850.29	Joback Method
dvisc	0.0000452	Paxs	909.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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