

Isophthalic acid, 8-chlorooctyl isobutyl ester

Inchi:	InChI=1S/C20H29ClO4/c1-16(2)15-25-20(23)18-11-9-10-17(14-18)19(22)24-13-8-6-4-3-5
InchiKey:	FMYRYFAHJCAYNJ-UHFFFAOYSA-N
Formula:	C20H29ClO4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)OCCCCCCCCCl)c1
Mol. weight [g/mol]:	368.89

Physical Properties

Property code	Value	Unit	Source
gf	-261.91	kJ/mol	Joback Method
hf	-741.69	kJ/mol	Joback Method
hfus	47.46	kJ/mol	Joback Method
hvap	85.36	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.236		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinsol	2719.00		NIST Webbook
tb	878.23	K	Joback Method
tc	1085.09	K	Joback Method
tf	513.34	K	Joback Method
vc	1.139	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.47	J/molxK	878.23	Joback Method
cpg	920.52	J/molxK	912.71	Joback Method
cpg	934.40	J/molxK	947.18	Joback Method
cpg	947.12	J/molxK	981.66	Joback Method
cpg	958.72	J/molxK	1016.14	Joback Method
cpg	969.21	J/molxK	1050.62	Joback Method
cpg	978.64	J/molxK	1085.09	Joback Method
dvisc	0.0005407	Paxs	513.34	Joback Method
dvisc	0.0002839	Paxs	574.15	Joback Method

dvisc	0.0001687	Paxs	634.97	Joback Method
dvisc	0.0001098	Paxs	695.78	Joback Method
dvisc	0.0000765	Paxs	756.60	Joback Method
dvisc	0.0000563	Paxs	817.41	Joback Method
dvisc	0.0000432	Paxs	878.23	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=U356386&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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