

Isophthalic acid, butyl 8-chlorooctyl ester

Inchi:	InChI=1S/C20H29ClO4/c1-2-3-14-24-19(22)17-11-10-12-18(16-17)20(23)25-15-9-7-5-4-6
InchiKey:	LISJPSGXBKACLE-UHFFFAOYSA-N
Formula:	C20H29ClO4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCl)c1
Mol. weight [g/mol]:	368.89

Physical Properties

Property code	Value	Unit	Source
gf	-259.47	kJ/mol	Joback Method
hf	-736.41	kJ/mol	Joback Method
hfus	50.98	kJ/mol	Joback Method
hvap	85.75	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.380		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpol	2768.00		NIST Webbook
tb	878.67	K	Joback Method
tc	1084.02	K	Joback Method
tf	528.34	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.96	J/molxK	878.67	Joback Method
cpg	919.93	J/molxK	912.90	Joback Method
cpg	933.75	J/molxK	947.12	Joback Method
cpg	946.44	J/molxK	981.35	Joback Method
cpg	958.03	J/molxK	1015.57	Joback Method
cpg	968.55	J/molxK	1049.80	Joback Method
cpg	978.02	J/molxK	1084.02	Joback Method
dvisc	0.0004842	Paxs	528.34	Joback Method
dvisc	0.0002709	Paxs	586.73	Joback Method

dvisc	0.0001684	Paxs	645.12	Joback Method
dvisc	0.0001132	Paxs	703.50	Joback Method
dvisc	0.0000809	Paxs	761.89	Joback Method
dvisc	0.0000607	Paxs	820.28	Joback Method
dvisc	0.0000473	Paxs	878.67	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=U356387&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
mccvol:	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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