Isophthalic acid, butyl 8-chloroctyl 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/mol×K	878.67	Joback Method
cpg	919.93	J/mol×K	912.90	Joback Method
cpg	933.75	J/mol×K	947.12	Joback Method
cpg	946.44	J/mol×K	981.35	Joback Method
cpg	958.03	J/mol×K	1015.57	Joback Method
cpg	968.55	J/mol×K	1049.80	Joback Method
cpg	978.02	J/mol×K	1084.02	Joback Method
dvisc	0.0004842	Pa×s	528.34	Joback Method
dvisc	0.0002709	Pa×s	586.73	Joback Method

dvisc	0.0001684	Pa×s	645.12	Joback Method
dvisc	0.0001132	Pa×s	703.50	Joback Method
dvisc	0.0000809	Pa×s	761.89	Joback Method
dvisc	0.0000607	Pa×s	820.28	Joback Method
dvisc	0.0000473	Pa×s	878.67	Joback Method

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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