

Isophthalic acid, butyl 6-chlorohexyl ester

Inchi:	InChI=1S/C18H25ClO4/c1-2-3-12-22-17(20)15-9-8-10-16(14-15)18(21)23-13-7-5-4-6-11-
InchiKey:	XUHCRUQCCKTKHC-UHFFFAOYSA-N
Formula:	C18H25ClO4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OCCCCC(Cl)C)c1
Mol. weight [g/mol]:	340.84

Physical Properties

Property code	Value	Unit	Source
gf	-276.31	kJ/mol	Joback Method
hf	-695.13	kJ/mol	Joback Method
hfus	45.80	kJ/mol	Joback Method
hvap	81.30	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.599		Crippen Method
mvol	267.840	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook
tb	832.91	K	Joback Method
tc	1037.04	K	Joback Method
tf	505.80	K	Joback Method
vc	1.032	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.39	J/molxK	832.91	Joback Method
cpg	802.92	J/molxK	866.93	Joback Method
cpg	816.38	J/molxK	900.95	Joback Method
cpg	828.80	J/molxK	934.97	Joback Method
cpg	840.20	J/molxK	968.99	Joback Method
cpg	850.59	J/molxK	1003.02	Joback Method
cpg	860.00	J/molxK	1037.04	Joback Method
dvisc	0.0005954	Paxs	505.80	Joback Method

dvisc	0.0003411	Paxs	560.32	Joback Method
dvisc	0.0002157	Paxs	614.84	Joback Method
dvisc	0.0001470	Paxs	669.36	Joback Method
dvisc	0.0001061	Paxs	723.87	Joback Method
dvisc	0.0000802	Paxs	778.39	Joback Method
dvisc	0.0000629	Paxs	832.91	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=U345879&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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