

Phthalic acid, butyl 4-chloro-2-methylphenyl ester

Inchi:	InChI=1S/C19H19ClO4/c1-3-4-11-23-18(21)15-7-5-6-8-16(15)19(22)24-17-10-9-14(20)1
InchiKey:	CGDSKNUQIGIZNG-UHFFFAOYSA-N
Formula:	C19H19ClO4
SMILES:	CCCCOC(=O)c1ccccc1C(=O)Oc1ccc(Cl)cc1C
Mol. weight [g/mol]:	346.81

Physical Properties

Property code	Value	Unit	Source
gf	-174.74	kJ/mol	Joback Method
hf	-502.18	kJ/mol	Joback Method
hfus	41.65	kJ/mol	Joback Method
hvap	87.12	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.825		Crippen Method
mvol	258.170	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2521.00		NIST Webbook
tb	892.43	K	Joback Method
tc	1122.94	K	Joback Method
tf	568.53	K	Joback Method
vc	0.981	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.88	J/molxK	892.43	Joback Method
cpg	757.38	J/molxK	930.85	Joback Method
cpg	768.61	J/molxK	969.27	Joback Method
cpg	778.59	J/molxK	1007.69	Joback Method
cpg	787.36	J/molxK	1046.11	Joback Method
cpg	794.94	J/molxK	1084.52	Joback Method
cpg	801.34	J/molxK	1122.94	Joback Method
dvisc	0.0003739	Paxs	568.53	Joback Method
dvisc	0.0002395	Paxs	622.51	Joback Method

dvisc	0.0001647	Paxs	676.50	Joback Method
dvisc	0.0001197	Paxs	730.48	Joback Method
dvisc	0.0000909	Paxs	784.46	Joback Method
dvisc	0.0000716	Paxs	838.45	Joback Method
dvisc	0.0000580	Paxs	892.43	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U356657&Units=SI

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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