

Pimelic acid, butyl 4-chloro-3-methylphenyl ester

Inchi:	InChI=1S/C18H25ClO4/c1-3-4-12-22-17(20)8-6-5-7-9-18(21)23-15-10-11-16(19)14(2)13
InchiKey:	QSKLCFHTZHDSNK-UHFFFAOYSA-N
Formula:	C18H25ClO4
SMILES:	CCCCOC(=O)CCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	340.84

Physical Properties

Property code	Value	Unit	Source
gf	-285.94	kJ/mol	Joback Method
hf	-706.60	kJ/mol	Joback Method
hfus	45.41	kJ/mol	Joback Method
hvap	81.96	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.848		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	2527.00		NIST Webbook
rinpol	2527.00		NIST Webbook
tb	837.89	K	Joback Method
tc	1042.84	K	Joback Method
tf	518.32	K	Joback Method
vc	1.032	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.46	J/molxK	837.89	Joback Method
cpg	801.91	J/molxK	872.05	Joback Method
cpg	815.29	J/molxK	906.21	Joback Method
cpg	827.62	J/molxK	940.37	Joback Method
cpg	838.91	J/molxK	974.53	Joback Method
cpg	849.18	J/molxK	1008.69	Joback Method
cpg	858.45	J/molxK	1042.84	Joback Method
dvisc	0.0005160	Paxs	518.32	Joback Method

dvisc	0.0003094	Paxs	571.58	Joback Method
dvisc	0.0002025	Paxs	624.84	Joback Method
dvisc	0.0001416	Paxs	678.10	Joback Method
dvisc	0.0001043	Paxs	731.37	Joback Method
dvisc	0.0000801	Paxs	784.63	Joback Method
dvisc	0.0000636	Paxs	837.89	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=U416683&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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