

Butyric acid, 2-phenyl-, 4-chlorophenyl ester

Inchi:	InChI=1S/C16H15ClO2/c1-2-15(12-6-4-3-5-7-12)16(18)19-14-10-8-13(17)9-11-14/h3-11,
InchiKey:	LYNMZXASBCHWCJ-UHFFFAOYSA-N
Formula:	C16H15ClO2
SMILES:	CCC(C(=O)Oc1ccc(Cl)cc1)c1ccccc1
Mol. weight [g/mol]:	274.74

Physical Properties

Property code	Value	Unit	Source
gf	50.74	kJ/mol	Joback Method
hf	-177.80	kJ/mol	Joback Method
hfus	28.35	kJ/mol	Joback Method
hvap	69.58	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.439		Crippen Method
mvol	208.460	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	737.10	K	Joback Method
tc	977.90	K	Joback Method
tf	422.52	K	Joback Method
vc	0.782	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.33	J/molxK	737.10	Joback Method
cpg	607.05	J/molxK	937.77	Joback Method
cpg	596.76	J/molxK	897.64	Joback Method
cpg	585.40	J/molxK	857.50	Joback Method
cpg	572.91	J/molxK	817.37	Joback Method
cpg	559.24	J/molxK	777.23	Joback Method
cpg	616.32	J/molxK	977.90	Joback Method
dvisc	0.0001031	Paxs	737.10	Joback Method

dvisc	0.0001325	Paxs	684.67	Joback Method
dvisc	0.0001774	Paxs	632.24	Joback Method
dvisc	0.0002504	Paxs	579.81	Joback Method
dvisc	0.0003785	Paxs	527.38	Joback Method
dvisc	0.0006268	Paxs	474.95	Joback Method
dvisc	0.0011764	Paxs	422.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406874&Units=SI
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

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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