

4-Bromobutyric acid, 2,3-dimethylphenyl ester

Inchi:	InChI=1S/C12H15BrO2/c1-9-5-3-6-11(10(9)2)15-12(14)7-4-8-13/h3,5-6H,4,7-8H2,1-2H3
InchiKey:	WJZUEQCZKNGYQR-UHFFFAOYSA-N
Formula:	C12H15BrO2
SMILES:	Cc1cccc(OC(=O)CCBr)c1C
Mol. weight [g/mol]:	271.15

Physical Properties

Property code	Value	Unit	Source
gf	-76.29	kJ/mol	Joback Method
hf	-295.89	kJ/mol	Joback Method
hfus	28.17	kJ/mol	Joback Method
hvap	61.50	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.384		Crippen Method
mcvol	181.120	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpola	1863.00		NIST Webbook
tb	653.05	K	Joback Method
tc	872.87	K	Joback Method
tf	408.42	K	Joback Method
vc	0.685	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.95	J/molxK	653.05	Joback Method
cpg	492.64	J/molxK	836.24	Joback Method
cpg	482.26	J/molxK	799.60	Joback Method
cpg	471.13	J/molxK	762.96	Joback Method
cpg	459.21	J/molxK	726.32	Joback Method
cpg	446.49	J/molxK	689.69	Joback Method
cpg	502.29	J/molxK	872.87	Joback Method
dvisc	0.0001702	Paxs	653.05	Joback Method
dvisc	0.0002092	Paxs	612.28	Joback Method

dvisc	0.0002649	Paxs	571.51	Joback Method
dvisc	0.0003477	Paxs	530.74	Joback Method
dvisc	0.0004776	Paxs	489.96	Joback Method
dvisc	0.0006949	Paxs	449.19	Joback Method
dvisc	0.0010897	Paxs	408.42	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=U354690&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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