4-Bromobutyric acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C10H9BrCl2O2/c11-5-1-2-10(14)15-7-3-4-8(12)9(13)6-7/h3-4,6H,1-2,5H2
InchiKey: JFERDTAWUDNKAE-UHFFFAOYSA-N
Formula: C10H9BrCl2O2
SMILES: O=C(CCCBr)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 311.99

Physical Properties

Property code	Value	Unit	Source
gf	-116.99	kJ/mol	Joback Method
hf	-286.09	kJ/mol	Joback Method
hfus	31.39	kJ/mol	Joback Method
hvap	65.81	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.074		Crippen Method
mcvol	177.420	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1942.00		NIST Webbook
tb	682.15	K	Joback Method
tc	916.45	K	Joback Method
tf	445.72	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.81	J/mol×K	682.15	Joback Method
cpg	424.66	J/mol×K	877.40	Joback Method
cpg	417.28	J/mol×K	838.35	Joback Method
cpg	409.23	J/mol×K	799.30	Joback Method
cpg	400.49	J/mol×K	760.25	Joback Method
cpg	391.02	J/mol×K	721.20	Joback Method
cpg	431.39	J/mol×K	916.45	Joback Method
dvisc	0.0001779	Pa×s	682.15	Joback Method
dvisc	0.0002164	Pa×s	642.75	Joback Method

dvisc	0.0002700	Pa×s	603.34	Joback Method
dvisc	0.0003475	Pa×s	563.93	Joback Method
dvisc	0.0004645	Pa×s	524.53	Joback Method
dvisc	0.0006509	Pa×s	485.12	Joback Method
dvisc	0.0009682	Pa×s	445.72	Joback Method

Sources

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=U307611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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