5-Bromovaleric acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C11H11BrCl2O2/c12-6-2-1-3-11(15)16-8-4-5-9(13)10(14)7-8/h4-5,7H,1-3,6H2
InchiKey: CVDJYPSWURIDQF-UHFFFAOYSA-N
Formula: C11H11BrCl2O2
SMILES: O=C(CCCCBr)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 326.01

Physical Properties

Property code	Value	Unit	Source
gf	-108.57	kJ/mol	Joback Method
hf	-306.73	kJ/mol	Joback Method
hfus	33.98	kJ/mol	Joback Method
hvap	68.04	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.464		Crippen Method
mcvol	191.510	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	2074.00		NIST Webbook
tb	705.03	K	Joback Method
tc	934.86	K	Joback Method
tf	456.99	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.09	J/mol×K	705.03	Joback Method
cpg	441.01	J/mol×K	743.33	Joback Method
cpg	451.16	J/mol×K	781.64	Joback Method
cpg	460.54	J/mol×K	819.94	Joback Method
cpg	469.20	J/mol×K	858.25	Joback Method
cpg	477.15	J/mol×K	896.55	Joback Method
cpg	484.43	J/mol×K	934.86	Joback Method
dvisc	0.0009031	Pa×s	456.99	Joback Method
dvisc	0.0005978	Pa×s	498.33	Joback Method

dvisc	0.0004215	Pa×s	539.67	Joback Method
dvisc	0.0003124	Pa×s	581.01	Joback Method
dvisc	0.0002409	Pa×s	622.35	Joback Method
dvisc	0.0001919	Pa×s	663.69	Joback Method
dvisc	0.0001570	Pa×s	705.03	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307646&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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