4-Bromobutyric acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C10H8BrCl3O2/c11-3-1-2-10(15)16-9-5-7(13)6(12)4-8(9)14/h4-5H,1-3H2
InchiKey: GQVNSYWBIORPPC-UHFFFAOYSA-N
Formula: C10H8BrCl3O2
SMILES: O=C(CCCBr)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 346.43

Physical Properties

Property code	Value	Unit	Source
gf	-138.55	kJ/mol	Joback Method
hf	-313.30	kJ/mol	Joback Method
hfus	35.19	kJ/mol	Joback Method
hvap	70.86	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.727		Crippen Method
mcvol	189.660	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	2147.00		NIST Webbook
tb	724.56	K	Joback Method
tc	962.23	K	Joback Method
tf	488.16	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.31	J/mol×K	724.56	Joback Method
cpg	438.18	J/mol×K	922.62	Joback Method
cpg	431.74	J/mol×K	883.01	Joback Method
cpg	424.65	J/mol×K	843.40	Joback Method
cpg	416.89	J/mol×K	803.78	Joback Method
cpg	408.46	J/mol×K	764.17	Joback Method
cpg	444.00	J/mol×K	962.23	Joback Method
dvisc	0.0001583	Pa×s	724.56	Joback Method
dvisc	0.0001900	Pa×s	685.16	Joback Method

dvisc	0.0002332	Pa×s	645.76	Joback Method
dvisc	0.0002939	Pa×s	606.36	Joback Method
dvisc	0.0003825	Pa×s	566.96	Joback Method
dvisc	0.0005177	Pa×s	527.56	Joback Method
dvisc	0.0007359	Pa×s	488.16	Joback Method

Sources

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=U354692&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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