4-Bromobutyric acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C10H7BrCl4O2/c11-3-1-2-7(16)17-10-6(13)4-5(12)8(14)9(10)15/h4H,1-3H2
InchiKey: YTEKABDCGWBMNM-UHFFFAOYSA-N
Formula: C10H7BrCl4O2
SMILES: O=C(CCCBr)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 380.88

Physical Properties

Property code	Value	Unit	Source
gf	-160.11	kJ/mol	Joback Method
hf	-340.51	kJ/mol	Joback Method
hfus	39.00	kJ/mol	Joback Method
hvap	75.91	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.381		Crippen Method
mcvol	201.900	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	2284.00		NIST Webbook
rinpol	2284.00		NIST Webbook
tb	766.97	K	Joback Method
tc	1007.70	K	Joback Method
tf	530.60	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.11	J/mol×K	766.97	Joback Method
cpg	450.20	J/mol×K	967.58	Joback Method
cpg	444.67	J/mol×K	927.46	Joback Method
cpg	438.51	J/mol×K	887.33	Joback Method
cpg	431.71	J/mol×K	847.21	Joback Method
cpg	424.25	J/mol×K	807.09	Joback Method
cpg	455.12	J/mol×K	1007.70	Joback Method
dvisc	0.0001399	Pa×s	766.97	Joback Method

dvisc	0.0001659	Pa×s	727.58	Joback Method
dvisc	0.0002007	Pa×s	688.18	Joback Method
dvisc	0.0002484	Pa×s	648.79	Joback Method
dvisc	0.0003161	Pa×s	609.39	Joback Method
dvisc	0.0004159	Pa×s	570.00	Joback Method
dvisc	0.0005699	Pa×s	530.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354693&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