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

Inchi: InChI=1S/C12H11BrCl4O2/c13-5-3-1-2-4-9(18)19-12-8(15)6-7(14)10(16)11(12)17/h6H,1

InchiKey: PESHYZZXVVLVSU-UHFFFAOYSA-N

Formula: C12H11BrCl4O2

SMILES: O=C(CCCCCBr)Oc1c(Cl)cc(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 408.93

Physical Properties

Property code	Value	Unit	Source
gf	-143.27	kJ/mol	Joback Method
hf	-381.79	kJ/mol	Joback Method
hfus	44.18	kJ/mol	Joback Method
hvap	80.36	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	6.161		Crippen Method
mcvol	230.080	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	2566.00		NIST Webbook
tb	812.73	K	Joback Method
tc	1045.28	K	Joback Method
tf	553.14	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.85	J/mol×K	812.73	Joback Method
cpg	558.45	J/mol×K	1006.52	Joback Method
cpg	551.96	J/mol×K	967.76	Joback Method
cpg	544.77	J/mol×K	929.01	Joback Method
cpg	536.87	J/mol×K	890.25	Joback Method
cpg	528.24	J/mol×K	851.49	Joback Method
cpg	564.27	J/mol×K	1045.28	Joback Method
dvisc	0.0001065	Pa×s	812.73	Joback Method
dvisc	0.0001275	Pa×s	769.47	Joback Method

dvisc	0.0001560	Pa×s	726.20	Joback Method
dvisc	0.0001959	Pa×s	682.94	Joback Method
dvisc	0.0002536	Pa×s	639.67	Joback Method
dvisc	0.0003408	Pa×s	596.41	Joback Method
dvisc	0.0004798	Pa×s	553.14	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354721&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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