6-Bromohexanoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C12H12BrCl3O2/c13-5-3-1-2-4-12(17)18-11-7-9(15)8(14)6-10(11)16/h6-7H,1-5

InchiKey: RFAYCUNNCKCRHH-UHFFFAOYSA-N

Formula: C12H12BrCl3O2

SMILES: O=C(CCCCCBr)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 374.49

Physical Properties

Property code	Value	Unit	Source
gf	-121.71	kJ/mol	Joback Method
hf	-354.58	kJ/mol	Joback Method
hfus	40.37	kJ/mol	Joback Method
hvap	75.31	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.508		Crippen Method
mcvol	217.840	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	2415.00		NIST Webbook
tb	770.32	K	Joback Method
tc	999.55	K	Joback Method
tf	510.70	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.67	J/mol×K	770.32	Joback Method
cpg	511.12	J/mol×K	808.52	Joback Method
cpg	520.77	J/mol×K	846.73	Joback Method
cpg	529.68	J/mol×K	884.93	Joback Method
cpg	537.85	J/mol×K	923.14	Joback Method
cpg	545.31	J/mol×K	961.34	Joback Method
cpg	552.10	J/mol×K	999.55	Joback Method
dvisc	0.0006276	Pa×s	510.70	Joback Method
dvisc	0.0004290	Pa×s	553.97	Joback Method

dvisc	0.0003099	Pa×s	597.24	Joback Method
dvisc	0.0002339	Pa×s	640.51	Joback Method
dvisc	0.0001830	Pa×s	683.78	Joback Method
dvisc	0.0001473	Pa×s	727.05	Joback Method
dvisc	0.0001216	Pa×s	770.32	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=U354720&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