6-Bromohexanoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C12H13BrCl2O2/c13-7-3-1-2-4-12(16)17-9-5-6-10(14)11(15)8-9/h5-6,8H,1-4,7
InchiKey: QOZCUULOIRYKJL-UHFFFAOYSA-N
Formula: C12H13BrCl2O2
SMILES: O=C(CCCCCBr)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 340.04

Physical Properties

Property code	Value	Unit	Source
gf	-100.15	kJ/mol	Joback Method
hf	-327.37	kJ/mol	Joback Method
hfus	36.56	kJ/mol	Joback Method
hvap	70.27	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.854		Crippen Method
mcvol	205.600	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	2186.00		NIST Webbook
rinpol	2186.00		NIST Webbook
tb	727.91	K	Joback Method
tc	953.69	K	Joback Method
tf	468.26	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.72	J/mol×K	727.91	Joback Method
cpg	492.26	J/mol×K	765.54	Joback Method
cpg	502.99	J/mol×K	803.17	Joback Method
cpg	512.92	J/mol×K	840.80	Joback Method
cpg	522.10	J/mol×K	878.43	Joback Method
cpg	530.56	J/mol×K	916.06	Joback Method
cpg	538.31	J/mol×K	953.69	Joback Method
dvisc	0.0008375	Pa×s	468.26	Joback Method

dvisc	0.0005461	Pa×s	511.53	Joback Method
dvisc	0.0003806	Pa×s	554.81	Joback Method
dvisc	0.0002795	Pa×s	598.09	Joback Method
dvisc	0.0002140	Pa×s	641.36	Joback Method
dvisc	0.0001695	Pa×s	684.63	Joback Method
dvisc	0.0001380	Pa×s	727.91	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=U307618&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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