

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

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

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