

6-Bromohexanoic acid, 2-propylphenyl ester

Inchi:	InChI=1S/C15H21BrO2/c1-2-8-13-9-5-6-10-14(13)18-15(17)11-4-3-7-12-16/h5-6,9-10H,2
InchiKey:	RERPNEREKHFAGY-UHFFFAOYSA-N
Formula:	C15H21BrO2
SMILES:	CCc1cccc1OC(=O)CCCCBr
Mol. weight [g/mol]:	313.23

Physical Properties

Property code	Value	Unit	Source
gf	-41.40	kJ/mol	Joback Method
hf	-346.34	kJ/mol	Joback Method
hfus	36.33	kJ/mol	Joback Method
hvap	67.51	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.500		Crippen Method
mvol	223.390	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
tb	716.71	K	Joback Method
tc	925.84	K	Joback Method
tf	429.71	K	Joback Method
vc	0.854	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.86	J/molxK	716.71	Joback Method
cpg	656.78	J/molxK	890.98	Joback Method
cpg	645.14	J/molxK	856.13	Joback Method
cpg	632.65	J/molxK	821.27	Joback Method
cpg	619.30	J/molxK	786.42	Joback Method
cpg	605.05	J/molxK	751.56	Joback Method
cpg	667.63	J/molxK	925.84	Joback Method
dvisc	0.0001192	Paxs	716.71	Joback Method

dvisc	0.0001508	Paxs	668.88	Joback Method
dvisc	0.0001978	Paxs	621.04	Joback Method
dvisc	0.0002716	Paxs	573.21	Joback Method
dvisc	0.0003950	Paxs	525.38	Joback Method
dvisc	0.0006192	Paxs	477.54	Joback Method
dvisc	0.0010728	Paxs	429.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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