

3-Bromobenzoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C15H20BrClO2/c16-14-9-7-8-13(12-14)15(18)19-11-6-4-2-1-3-5-10-17/h7-9,12
InchiKey: CMHBCXFMGCTGMY-UHFFFAOYSA-N
Formula: C15H20BrClO2
SMILES: O=C(OCCCCCCCCCl)c1cccc(Br)c1
Mol. weight [g/mol]: 347.68

Physical Properties

Property code	Value	Unit	Source
gf	-53.33	kJ/mol	Joback Method
hf	-362.08	kJ/mol	Joback Method
hfus	40.53	kJ/mol	Joback Method
hvap	71.90	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.185		Crippen Method
mvol	235.630	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
tb	754.14	K	Joback Method
tc	966.59	K	Joback Method
tf	459.63	K	Joback Method
vc	0.902	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.40	J/molxK	754.14	Joback Method
cpg	630.50	J/molxK	789.55	Joback Method
cpg	643.67	J/molxK	824.96	Joback Method
cpg	655.95	J/molxK	860.36	Joback Method
cpg	667.38	J/molxK	895.77	Joback Method
cpg	678.01	J/molxK	931.18	Joback Method
cpg	687.86	J/molxK	966.59	Joback Method
dvisc	0.0009013	Paxs	459.63	Joback Method

dvisc	0.0005300	Paxs	508.71	Joback Method
dvisc	0.0003422	Paxs	557.80	Joback Method
dvisc	0.0002371	Paxs	606.88	Joback Method
dvisc	0.0001736	Paxs	655.97	Joback Method
dvisc	0.0001327	Paxs	705.06	Joback Method
dvisc	0.0001051	Paxs	754.14	Joback Method

Sources

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=U355187&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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