

5-Bromovaleric acid, 2-naphthyl ester

Inchi:	InChI=1S/C15H15BrO2/c16-10-4-3-7-15(17)18-14-9-8-12-5-1-2-6-13(12)11-14/h1-2,5-6,8
InchiKey:	SSXPSKQYEAPOEG-UHFFFAOYSA-N
Formula:	C15H15BrO2
SMILES:	O=C(CCCCBBr)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	307.18

Physical Properties

Property code	Value	Unit	Source
gf	65.25	kJ/mol	Joback Method
hf	-155.27	kJ/mol	Joback Method
hfus	33.35	kJ/mol	Joback Method
hvap	69.15	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.310		Crippen Method
mcvol	203.930	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinsol	2287.00		NIST Webbook
tb	735.69	K	Joback Method
tc	968.11	K	Joback Method
tf	462.41	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.36	J/molxK	735.69	Joback Method
cpg	535.85	J/molxK	774.43	Joback Method
cpg	548.36	J/molxK	813.16	Joback Method
cpg	559.97	J/molxK	851.90	Joback Method
cpg	570.76	J/molxK	890.64	Joback Method
cpg	580.80	J/molxK	929.37	Joback Method
cpg	590.17	J/molxK	968.11	Joback Method
dvisc	0.0011517	Paxs	462.41	Joback Method
dvisc	0.0007723	Paxs	507.96	Joback Method

dvisc	0.0005531	Paxs	553.50	Joback Method
dvisc	0.0004168	Paxs	599.05	Joback Method
dvisc	0.0003269	Paxs	644.60	Joback Method
dvisc	0.0002647	Paxs	690.14	Joback Method
dvisc	0.0002200	Paxs	735.69	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=U307648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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