

6-Bromohexanoic acid, oct-3-en-2-yl ester

Inchi:	InChI=1S/C14H25BrO2/c1-3-4-5-7-10-13(2)17-14(16)11-8-6-9-12-15/h7,10,13H,3-6,8-9,
InchiKey:	OAYIJFZMPRIJHZ-JXMROGBWSA-N
Formula:	C14H25BrO2
SMILES:	CCCCC=CC(C)OC(=O)CCCCBr
Mol. weight [g/mol]:	305.25

Physical Properties

Property code	Value	Unit	Source
gf	-74.82	kJ/mol	Joback Method
hf	-438.82	kJ/mol	Joback Method
hfus	36.77	kJ/mol	Joback Method
hvap	61.92	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.620		Crippen Method
mcvol	228.760	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
tb	665.89	K	Joback Method
tc	854.11	K	Joback Method
tf	359.42	K	Joback Method
vc	0.879	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.57	J/molxK	665.89	Joback Method
cpg	612.33	J/molxK	697.26	Joback Method
cpg	627.29	J/molxK	728.63	Joback Method
cpg	641.49	J/molxK	760.00	Joback Method
cpg	654.95	J/molxK	791.37	Joback Method
cpg	667.71	J/molxK	822.74	Joback Method
cpg	679.80	J/molxK	854.11	Joback Method
dvisc	0.0020410	Paxs	359.42	Joback Method

dvisc	0.0009218	Paxs	410.50	Joback Method
dvisc	0.0004965	Paxs	461.58	Joback Method
dvisc	0.0003025	Paxs	512.65	Joback Method
dvisc	0.0002016	Paxs	563.73	Joback Method
dvisc	0.0001437	Paxs	614.81	Joback Method
dvisc	0.0001079	Paxs	665.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299290&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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