

11-Bromoundecanoic acid

Other names:	Undecanoic acid, 11-bromo-
Inchi:	InChI=1S/C11H21BrO2/c12-10-8-6-4-2-1-3-5-7-9-11(13)14/h1-10H2,(H,13,14)
InchiKey:	IUDGNRWYNOEIKF-UHFFFAOYSA-N
Formula:	C11H21BrO2
SMILES:	O=C(O)CCCCCCCCCBr
Mol. weight [g/mol]:	265.19
CAS:	2834-05-1

Physical Properties

Property code	Value	Unit	Source
gf	-209.68	kJ/mol	Joback Method
hf	-508.85	kJ/mol	Joback Method
hfus	35.22	kJ/mol	Joback Method
hvap	69.94	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.977		Crippen Method
mcvol	190.790	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
tb	663.29	K	Joback Method
tc	841.15	K	Joback Method
tf	384.28	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.45	J/mol×K	663.29	Joback Method
cpg	506.73	J/mol×K	692.93	Joback Method
cpg	518.42	J/mol×K	722.58	Joback Method
cpg	529.54	J/mol×K	752.22	Joback Method
cpg	540.12	J/mol×K	781.87	Joback Method
cpg	550.18	J/mol×K	811.51	Joback Method
cpg	559.75	J/mol×K	841.15	Joback Method
dvisc	0.0033566	Pa×s	384.28	Joback Method

dvisc	0.0012221	Pa×s	430.78	Joback Method
dvisc	0.0005418	Pa×s	477.28	Joback Method
dvisc	0.0002775	Pa×s	523.78	Joback Method
dvisc	0.0001585	Pa×s	570.29	Joback Method
dvisc	0.0000985	Pa×s	616.79	Joback Method
dvisc	0.0000655	Pa×s	663.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.70	K	0.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2834051&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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