Nonanoic acid, 2-bromoethyl ester

Other names: ethyl 2-bromononan-1-oate
Inchi: InChI=1S/C11H21BrO2/c1-3-5-6-7-8-9-10(12)11(13)14-4-2/h10H,3-9H2,1-2H3
InchiKey: QARKIRQNOLQDFJ-UHFFFAOYSA-N
Formula: C11H21BrO2
SMILES: CCCCCCCC(Br)C(=O)OCC
Mol. weight [g/mol]: 265.19
CAS: 7425-60-7

Physical Properties

Property code	Value	Unit	Source
gf	-180.30	kJ/mol	Joback Method
hf	-494.12	kJ/mol	Joback Method
hfus	28.80	kJ/mol	Joback Method
hvap	55.28	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.674		Crippen Method
mcvol	190.790	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook
tb	593.09	K	Joback Method
tc	779.97	K	Joback Method
tf	330.69	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.31	J/mol×K	593.09	Joback Method
cpg	528.64	J/mol×K	748.82	Joback Method
cpg	516.68	J/mol×K	717.68	Joback Method
cpg	504.08	J/mol×K	686.53	Joback Method
cpg	490.82	J/mol×K	655.38	Joback Method
cpg	476.91	J/mol×K	624.24	Joback Method

cpg	539.99	J/mol×K	779.97	Joback Method
dvisc	0.0001832	Pa×s	593.09	Joback Method
dvisc	0.0002408	Pa×s	549.36	Joback Method
dvisc	0.0003319	Pa×s	505.62	Joback Method
dvisc	0.0004860	Pa×s	461.89	Joback Method
dvisc	0.0007709	Pa×s	418.16	Joback Method
dvisc	0.0013618	Pa×s	374.42	Joback Method
dvisc	0.0027963	Pa×s	330.69	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=C7425607&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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