

Nonyl 2-bromobutanoate

Inchi:	InChI=1S/C13H25BrO2/c1-3-5-6-7-8-9-10-11-16-13(15)12(14)4-2/h12H,3-11H2,1-2H3
InchiKey:	QLHKAJYBOHBZQL-UHFFFAOYSA-N
Formula:	C13H25BrO2
SMILES:	CCCCCCCCCOC(=O)C(Br)CC
Mol. weight [g/mol]:	293.24

Physical Properties

Property code	Value	Unit	Source
gf	-163.46	kJ/mol	Joback Method
hf	-535.40	kJ/mol	Joback Method
hfus	33.98	kJ/mol	Joback Method
hvap	59.73	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.454		Crippen Method
mvol	218.970	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	638.85	K	Joback Method
tc	822.28	K	Joback Method
tf	353.23	K	Joback Method
vc	0.844	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.89	J/molxK	638.85	Joback Method
cpg	636.33	J/molxK	791.71	Joback Method
cpg	623.47	J/molxK	761.14	Joback Method
cpg	609.91	J/molxK	730.56	Joback Method
cpg	595.63	J/molxK	699.99	Joback Method
cpg	580.63	J/molxK	669.42	Joback Method
cpg	648.53	J/molxK	822.28	Joback Method
dvisc	0.0001429	Paxs	638.85	Joback Method

dvisc	0.0001891	Paxs	591.25	Joback Method
dvisc	0.0002630	Paxs	543.64	Joback Method
dvisc	0.0003895	Paxs	496.04	Joback Method
dvisc	0.0006271	Paxs	448.44	Joback Method
dvisc	0.0011305	Paxs	400.83	Joback Method
dvisc	0.0023891	Paxs	353.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R23483&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

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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