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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.89	J/mol×K	638.85	Joback Method
cpg	580.63	J/mol×K	669.42	Joback Method
cpg	595.63	J/mol×K	699.99	Joback Method
cpg	609.91	J/mol×K	730.56	Joback Method
cpg	623.47	J/mol×K	761.14	Joback Method
cpg	636.33	J/mol×K	791.71	Joback Method
cpg	648.53	J/mol×K	822.28	Joback Method
dvisc	0.0023891	Pa×s	353.23	Joback Method

dvisc	0.0011305	Pa×s	400.83	Joback Method
dvisc	0.0006271	Pa×s	448.44	Joback Method
dvisc	0.0003895	Pa×s	496.04	Joback Method
dvisc	0.0002630	Pa×s	543.64	Joback Method
dvisc	0.0001891	Pa×s	591.25	Joback Method
dvisc	0.0001429	Pa×s	638.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R23483&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume