

Nonyl 2-bromopropanoate

Inchi:	InChI=1S/C12H23BrO2/c1-3-4-5-6-7-8-9-10-15-12(14)11(2)13/h11H,3-10H2,1-2H3
InchiKey:	RYJOCSXNXWJISS-UHFFFAOYSA-N
Formula:	C12H23BrO2
SMILES:	CCCCCCCCCOC(=O)C(C)Br
Mol. weight [g/mol]:	279.21

Physical Properties

Property code	Value	Unit	Source
gf	-171.88	kJ/mol	Joback Method
hf	-514.76	kJ/mol	Joback Method
hfus	31.39	kJ/mol	Joback Method
hvap	57.51	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.064		Crippen Method
mvol	204.880	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
tb	615.97	K	Joback Method
tc	800.98	K	Joback Method
tf	341.96	K	Joback Method
vc	0.787	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.85	J/mol×K	615.97	Joback Method
cpg	581.90	J/mol×K	770.15	Joback Method
cpg	569.46	J/mol×K	739.31	Joback Method
cpg	556.34	J/mol×K	708.48	Joback Method
cpg	542.55	J/mol×K	677.64	Joback Method
cpg	528.06	J/mol×K	646.81	Joback Method
cpg	593.71	J/mol×K	800.98	Joback Method
dvisc	0.0001621	Paxs	615.97	Joback Method

dvisc	0.0002139	Paxs	570.30	Joback Method
dvisc	0.0002961	Paxs	524.63	Joback Method
dvisc	0.0004362	Paxs	478.97	Joback Method
dvisc	0.0006973	Paxs	433.30	Joback Method
dvisc	0.0012447	Paxs	387.63	Joback Method
dvisc	0.0025939	Paxs	341.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R23497&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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