

Butanoic acid, 2-bromo-, pentyl ester

Other names:	Pentyl 2-bromobutanoate
Inchi:	InChI=1S/C9H17BrO2/c1-3-5-6-7-12-9(11)8(10)4-2/h8H,3-7H2,1-2H3
InchiKey:	TYNCRXMYKJONLT-UHFFFAOYSA-N
Formula:	C9H17BrO2
SMILES:	CCCCCOC(=O)C(Br)CC
Mol. weight [g/mol]:	237.13

Physical Properties

Property code	Value	Unit	Source
gf	-197.14	kJ/mol	Joback Method
hf	-452.84	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	50.83	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.893		Crippen Method
mvol	162.610	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
tb	547.33	K	Joback Method
tc	738.62	K	Joback Method
tf	308.15	K	Joback Method
vc	0.620	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.10	J/molxK	547.33	Joback Method
cpg	379.22	J/molxK	579.21	Joback Method
cpg	391.74	J/molxK	611.09	Joback Method
cpg	403.67	J/molxK	642.98	Joback Method
cpg	415.02	J/molxK	674.86	Joback Method
cpg	425.81	J/molxK	706.74	Joback Method
cpg	436.04	J/molxK	738.62	Joback Method

dvisc	0.0031707	Paxs	308.15	Joback Method
dvisc	0.0015948	Paxs	348.01	Joback Method
dvisc	0.0009238	Paxs	387.88	Joback Method
dvisc	0.0005925	Paxs	427.74	Joback Method
dvisc	0.0004099	Paxs	467.60	Joback Method
dvisc	0.0003004	Paxs	507.47	Joback Method
dvisc	0.0002304	Paxs	547.33	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U131818&Units=SI

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
mvol:	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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