

Pentanedioic acid, 2-bromo-, diethyl ester

Inchi:	InChI=1S/C9H15BrO4/c1-3-13-8(11)6-5-7(10)9(12)14-4-2/h7H,3-6H2,1-2H3
InchiKey:	OXJSWZSWGJACGU-UHFFFAOYSA-N
Formula:	C9H15BrO4
SMILES:	CCOC(=O)CCC(Br)C(=O)OCC
Mol. weight [g/mol]:	267.12
CAS:	7209-00-9

Physical Properties

Property code	Value	Unit	Source
gf	-431.06	kJ/mol	Joback Method
hf	-697.64	kJ/mol	Joback Method
hfus	26.40	kJ/mol	Joback Method
hvap	59.99	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.656		Crippen Method
mcvol	170.050	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
tb	623.62	K	Joback Method
tc	821.10	K	Joback Method
tf	380.31	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.44	J/molxK	623.62	Joback Method
cpg	419.39	J/molxK	656.53	Joback Method
cpg	430.73	J/molxK	689.45	Joback Method
cpg	441.48	J/molxK	722.36	Joback Method
cpg	451.63	J/molxK	755.27	Joback Method
cpg	461.18	J/molxK	788.19	Joback Method
cpg	470.13	J/molxK	821.10	Joback Method
dvisc	0.0017612	Paxs	380.31	Joback Method
dvisc	0.0010043	Paxs	420.86	Joback Method

dvisc	0.0006321	Paxs	461.41	Joback Method
dvisc	0.0004288	Paxs	501.97	Joback Method
dvisc	0.0003082	Paxs	542.52	Joback Method
dvisc	0.0002320	Paxs	583.07	Joback Method
dvisc	0.0001811	Paxs	623.62	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=C7209009&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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