

Ethyl bromodifluoroacetate

Other names:	Acetic acid, bromodifluoro-, ethyl ester
Inchi:	InChI=1S/C4H5BrF2O2/c1-2-9-3(8)4(5,6)7/h2H2,1H3
InchiKey:	IRSJDVYTJUCXRV-UHFFFAOYSA-N
Formula:	C4H5BrF2O2
SMILES:	CCOC(=O)C(F)(F)Br
Mol. weight [g/mol]:	202.98
CAS:	667-27-6

Physical Properties

Property code	Value	Unit	Source
gf	-623.58	kJ/mol	Joback Method
hf	-745.33	kJ/mol	Joback Method
hfus	12.93	kJ/mol	Joback Method
hvap	37.16	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.537		Crippen Method
mcvol	95.700	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
tb	428.68	K	Joback Method
tc	618.99	K	Joback Method
tf	270.40	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.44	J/molxK	428.68	Joback Method
cpg	185.77	J/molxK	460.40	Joback Method
cpg	192.67	J/molxK	492.12	Joback Method
cpg	199.14	J/molxK	523.83	Joback Method
cpg	205.22	J/molxK	555.55	Joback Method
cpg	210.91	J/molxK	587.27	Joback Method
cpg	216.24	J/molxK	618.99	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.00	K	93.30	NIST Webbook
tbrp	385.20	K	93.30	NIST Webbook

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=C667276&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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