

ethyl 4-bromocrotonate

Inchi:	InChI=1S/C6H9BrO2/c1-2-9-6(8)4-3-5-7/h3-4H,2,5H2,1H3
InchiKey:	FHGRPBSDPBRTLS-UHFFFAOYSA-N
Formula:	C6H9BrO2
SMILES:	CCOC(=O)C=CCBr
Mol. weight [g/mol]:	193.04
CAS:	6065-32-3

Physical Properties

Property code	Value	Unit	Source
gf	-139.74	kJ/mol	Joback Method
hf	-268.42	kJ/mol	Joback Method
hfus	19.57	kJ/mol	Joback Method
hvap	44.50	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.501		Crippen Method
mcvol	116.040	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
tb	483.29	K	Joback Method
tc	687.04	K	Joback Method
tf	284.26	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.83	J/molxK	483.29	Joback Method
cpg	227.03	J/molxK	517.25	Joback Method
cpg	235.76	J/molxK	551.21	Joback Method
cpg	244.02	J/molxK	585.16	Joback Method
cpg	251.85	J/molxK	619.12	Joback Method
cpg	259.25	J/molxK	653.08	Joback Method
cpg	266.25	J/molxK	687.04	Joback Method
dvisc	0.0024279	Paxs	284.26	Joback Method
dvisc	0.0013964	Paxs	317.43	Joback Method

dvisc	0.0008917	Paxs	350.60	Joback Method
dvisc	0.0006154	Paxs	383.77	Joback Method
dvisc	0.0004505	Paxs	416.95	Joback Method
dvisc	0.0003453	Paxs	450.12	Joback Method
dvisc	0.0002745	Paxs	483.29	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=C6065323&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
mccvol:	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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