

Iso-butyl iso-cyanato acetate

Inchi: InChI=1S/C7H11NO3/c1-6(2)4-11-7(10)3-8-5-9/h6H,3-4H2,1-2H3
InchiKey: OWODJWQSTODZEF-UHFFFAOYSA-N
Formula: C7H11NO3
SMILES: CC(C)COC(=O)CN=C=O
Mol. weight [g/mol]: 157.17
CAS: 89775-61-1

Physical Properties

Property code	Value	Unit	Source
hf	-443.30	kJ/mol	Joback Method
hvac	49.48	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	0.521		Crippen Method
mcvol	124.180	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
tb	502.08	K	Joback Method
tc	692.47	K	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=C89775611&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

hf: Enthalpy of formation at standard conditions
hvac: 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

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