2-butenamide

Inchi: InChI=1S/C4H7NO/c1-2-3-4(5)6/h2-3H,1H3,(H2,5,6)
InchiKey: NQQRXZOPZBKCNF-UHFFFAOYSA-N
Formula: C4H7NO
SMILES: CC=CC(N)=O
Mol. weight [g/mol]: 85.10
CAS: 23350-58-5

Physical Properties

Property code	Value	Unit	Source
affp	887.10	kJ/mol	NIST Webbook
basg	856.10	kJ/mol	NIST Webbook
gf	0.55	kJ/mol	Joback Method
hf	-87.46	kJ/mol	Joback Method
hfus	13.11	kJ/mol	Joback Method
hvap	41.84	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	0.048		Crippen Method
mcvol	74.470	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
tb	421.48	K	Joback Method
tc	627.04	K	Joback Method
tf	262.95	K	Joback Method
vc	0.275	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.13	J/mol×K	421.48	Joback Method
cpg	143.74	J/mol×K	455.74	Joback Method
cpg	150.91	J/mol×K	490.00	Joback Method
cpg	157.67	J/mol×K	524.26	Joback Method
cpg	164.04	J/mol×K	558.52	Joback Method
cpg	170.03	J/mol×K	592.78	Joback Method
cpg	175.67	J/mol×K	627.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C23350585&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume