(E)-N-Isopropyl-2-butenamide

Inchi: InChI=1S/C7H13NO/c1-4-5-7(9)8-6(2)3/h4-6H,1-3H3,(H,8,9)/b5-4+
InchiKey: PMYOYDPRILKMKB-SNAWJCMRSA-N
Formula: C7H13NO
SMILES: CC=CC(=O)NC(C)C
Mol. weight [g/mol]: 127.18

Physical Properties

Property code	Value	Unit	Source
gf	46.31	kJ/mol	Joback Method
hf	-134.98	kJ/mol	Joback Method
hfus	17.26	kJ/mol	Joback Method
hvap	43.93	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.087		Crippen Method
mcvol	116.740	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook
tb	467.32	K	Joback Method
tc	660.45	K	Joback Method
tf	251.16	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.81	J/mol×K	467.32	Joback Method
cpg	254.70	J/mol×K	499.51	Joback Method
cpg	265.97	J/mol×K	531.70	Joback Method
cpg	276.67	J/mol×K	563.89	Joback Method
cpg	286.80	J/mol×K	596.07	Joback Method
cpg	296.40	J/mol×K	628.26	Joback Method
cpg	305.49	J/mol×K	660.45	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=R644265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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