trans 2-Nonenoic acid amide

Inchi: InChI=1S/C9H17NO/c1-2-3-4-5-6-7-8-9(10)11/h7-8H,2-6H2,1H3,(H2,10,11)/b8-7+
InchiKey: PRCOWBGHTCNVDZ-BQYQJAHWSA-N
Formula: C9H17NO
SMILES: CCCCCCC=CC(N)=O
Mol. weight [g/mol]: 155.24
CAS: 14952-05-7

Physical Properties

Property code	Value	Unit	Source
gf	42.65	kJ/mol	Joback Method
hf	-190.66	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	52.97	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.998		Crippen Method
mcvol	144.920	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
tb	535.88	K	Joback Method
tc	728.96	K	Joback Method
tf	319.30	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.92	J/mol×K	535.88	Joback Method
cpg	354.16	J/mol×K	568.06	Joback Method
cpg	366.73	J/mol×K	600.24	Joback Method
cpg	378.65	J/mol×K	632.42	Joback Method
cpg	389.95	J/mol×K	664.60	Joback Method
cpg	400.66	J/mol×K	696.78	Joback Method
cpg	410.81	J/mol×K	728.96	Joback Method
hsubt	111.90	kJ/mol	388.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14952057&Units=SI
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

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
hsubt:	Enthalpy of sublimation at a given temperature
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