4,6(1H,5H)-Pyrimidinedione, 5-ethyldihydro-5-(1-methylpropyl)-2-thioxo-

Other names: 5-(sec-butyl)-5-ethyldihydro-2-thioxopyrimidine-4,6(1H,5H)-dione
Inchi: InChI=1S/C10H16N2O2S/c1-4-6(3)10(5-2)7(13)11-9(15)12-8(10)14/h6H,4-5H2,1-3H3,(H
InchiKey: IDELNEDBPWKHGK-UHFFFAOYSA-N
Formula: C10H16N2O2S
SMILES: CCC(C)C1(CC)C(=O)NC(=S)NC1=O
Mol. weight [g/mol]: 228.31
CAS: 2095-57-0

Physical Properties

Property code	Value	Unit	Source
gf	70.93	kJ/mol	Joback Method
hf	-270.13	kJ/mol	Joback Method
hfus	27.90	kJ/mol	Joback Method
hvap	66.23	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	0.960		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	1790.00		NIST Webbook
tb	752.93	K	Joback Method
tc	1014.20	K	Joback Method
tf	628.91	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.85	J/mol×K	752.93	Joback Method
cpg	510.56	J/mol×K	796.48	Joback Method
cpg	526.56	J/mol×K	840.02	Joback Method
cpg	541.93	J/mol×K	883.57	Joback Method
cpg	556.77	J/mol×K	927.11	Joback Method
cpg	571.16	J/mol×K	970.66	Joback Method
cpg	585.20	J/mol×K	1014.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2095570&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
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