

Ethypicone

Other names:	3,3-Diethyl-5-methyl-2,4(1H,3H)-pyridinedione 3,3-Diethyl-5-methyl-1,2,3,4-tetrahydropyridin-2,4-dione Deshydromethylprylon Dehydromethylprylon Methylpersedon 5-Methylpyrithyldione Deshydromethypylon Methypylon M (OH, -H2O)
Inchi:	InChI=1S/C10H15NO2/c1-4-10(5-2)8(12)7(3)6-11-9(10)13/h6H,4-5H2,1-3H3,(H,11,13)
InchiKey:	WELBEQNHUMMKEL-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	CCC1(CC)C(=O)NC=C(C)C1=O
Mol. weight [g/mol]:	181.23
CAS:	467-90-3

Physical Properties

Property code	Value	Unit	Source
gf	-84.86	kJ/mol	Joback Method
hf	-371.45	kJ/mol	Joback Method
hfus	16.64	kJ/mol	Joback Method
hvap	53.34	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.396		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1540.00		NIST Webbook
tb	636.32	K	Joback Method
tc	879.83	K	Joback Method
tf	488.49	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	394.59	J/mol×K	636.32	Joback Method
cpg	411.40	J/mol×K	676.90	Joback Method
cpg	427.46	J/mol×K	717.49	Joback Method
cpg	442.81	J/mol×K	758.07	Joback Method
cpg	457.52	J/mol×K	798.66	Joback Method
cpg	471.64	J/mol×K	839.24	Joback Method
cpg	485.21	J/mol×K	879.83	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=C467903&Units=SI

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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