

3,3-Diethyl-5-methyl-1,2,3,4-tetrahydropyridin-2,4-

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]:	181.24

Physical Properties

Property code	Value	Unit	Source
hfus	16.64	kJ/mol	Joback Method
ie	8.50	eV	Cheméo Relay (1.0)
log10ws	-1.72		Cheméo Relay (1.0)
logp	1.396		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
tf	411.62	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C467903&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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