PYRROLIDIN-2-ONE, 5-[2-BUTYRYLETHYL]-

Other names: «alpha»-Pyrrolidone, 5-[2-butyrylethyl]-
5-[2-butyrylethyl]pyrrolidin-2-one
Inchi: InChI=1S/C10H17NO2/c1-2-3-9(12)6-4-8-5-7-10(13)11-8/h8H,2-7H2,1H3,(H,11,13)
InchiKey: BAUFTTJSFZLNJB-UHFFFAOYSA-N
Formula: C10H17NO2
SMILES: CCCC(=O)CCC1CCC(=O)N1
Mol. weight [g/mol]: 183.25

Physical Properties

Property code	Value	Unit	Source
hf	-441.90	kJ/mol	Cheméo Relay (1.0)
hfus	26.29	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Cheméo Relay (1.0)
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-0.99		Cheméo Relay (1.0)
logp	1.414		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
rinpol	1229.00		NIST Webbook
tb	579.96	K	Cheméo Relay (1.0)
tc	782.19	K	Cheméo Relay (1.0)
tf	351.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.62	J/mol×K	613.72	Joback Method
cpg	424.23	J/mol×K	650.08	Joback Method
cpg	439.94	J/mol×K	686.45	Joback Method
cpg	454.76	J/mol×K	722.81	Joback Method
cpg	468.67	J/mol×K	759.17	Joback Method
cpg	481.68	J/mol×K	795.54	Joback Method
cpg	493.79	J/mol×K	831.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117155756&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point