

Cropropamide

Other names:

2-Butenamide, N-[1-[(dimethylamino)carbonyl]propyl]-N-propyl-
2-Butenamide, N1-(1-[(dimethylamino)carbonyl]propyl)-N1-propyl
N-(1-[(Dimethylamino)carbonyl]propyl)-n-propyl-2-butenamide
Cropropamidum
Crotonamide, N-(1-(dimethylcarbamoyl)propyl)-N-propyl-

Inchi: InChI=1S/C13H24N2O2/c1-6-9-12(16)15(10-7-2)11(8-3)13(17)14(4)5/h6,9,11H,7-8,10H2**InchiKey:** CYZWCBZIBJLKCV-RMKNXTFCSA-N**Formula:** C13H24N2O2**SMILES:** CC=CC(=O)N(CCC)C(CC)C(=O)N(C)C**Mol. weight [g/mol]:** 240.34**CAS:** 633-47-6

Physical Properties

Property code	Value	Unit	Source
gf	100.08	kJ/mol	Joback Method
hf	-289.81	kJ/mol	Joback Method
hfus	35.34	kJ/mol	Joback Method
hvap	61.68	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.668		Crippen Method
mcvol	212.830	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	1737.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1715.00		NIST Webbook
tb	633.18	K	Joback Method
tc	816.51	K	Joback Method
tf	380.99	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.41	J/molxK	633.18	Joback Method

cpg	585.47	J/mol×K	663.73	Joback Method
cpg	600.66	J/mol×K	694.29	Joback Method
cpg	615.02	J/mol×K	724.84	Joback Method
cpg	628.60	J/mol×K	755.40	Joback Method
cpg	641.44	J/mol×K	785.95	Joback Method
cpg	653.57	J/mol×K	816.51	Joback Method

Sources

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=C633476&Units=SI
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
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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