

Propanamide, 2-methyl-N-ethyl-N-hept-2-yl-

Inchi:	InChI=1S/C13H27NO/c1-6-8-9-10-12(5)14(7-2)13(15)11(3)4/h11-12H,6-10H2,1-5H3
InchiKey:	ZQGYWDLOBUNMIR-UHFFFAOYSA-N
Formula:	C13H27NO
SMILES:	CCCCC(C)N(CC)C(=O)C(C)C
Mol. weight [g/mol]:	213.36

Physical Properties

Property code	Value	Unit	Source
gf	35.56	kJ/mol	Joback Method
hf	-367.26	kJ/mol	Joback Method
hfus	27.00	kJ/mol	Joback Method
hvap	52.55	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.460		Crippen Method
mcvol	205.580	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	1727.00		NIST Webbook
rinpol	1727.00		NIST Webbook
tb	562.27	K	Joback Method
tc	735.96	K	Joback Method
tf	288.67	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.14	J/mol×K	562.27	Joback Method
cpg	541.88	J/mol×K	591.22	Joback Method
cpg	558.83	J/mol×K	620.17	Joback Method
cpg	574.99	J/mol×K	649.11	Joback Method
cpg	590.40	J/mol×K	678.06	Joback Method
cpg	605.07	J/mol×K	707.01	Joback Method
cpg	619.05	J/mol×K	735.96	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=U415344&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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