

But-2-enamide, N-decyl-N-methyl-3-methyl-

Inchi:	InChI=1S/C16H31NO/c1-5-6-7-8-9-10-11-12-13-17(4)16(18)14-15(2)3/h14H,5-13H2,1-4H
InchiKey:	BBXLRSKXRIPTNT-UHFFFAOYSA-N
Formula:	C16H31NO
SMILES:	CCCCCCCCCN(C)C(=O)C=C(C)C
Mol. weight [g/mol]:	253.42

Physical Properties

Property code	Value	Unit	Source
gf	137.37	kJ/mol	Joback Method
hf	-311.19	kJ/mol	Joback Method
hfus	40.71	kJ/mol	Joback Method
hvap	60.04	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.552		Crippen Method
mvol	243.550	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	1925.00		NIST Webbook
tb	635.83	K	Joback Method
tc	809.30	K	Joback Method
tf	333.44	K	Joback Method
vc	0.936	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.66	J/mol×K	635.83	Joback Method
cpg	682.89	J/mol×K	664.74	Joback Method
cpg	700.25	J/mol×K	693.65	Joback Method
cpg	716.79	J/mol×K	722.57	Joback Method
cpg	732.54	J/mol×K	751.48	Joback Method
cpg	747.55	J/mol×K	780.39	Joback Method
cpg	761.84	J/mol×K	809.30	Joback Method

Sources

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=U308238&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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