

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

Inchi:	InChI=1S/C19H37NO/c1-5-7-9-11-13-15-20(19(21)17-18(3)4)16-14-12-10-8-6-2/h17H,5-
InchiKey:	UGCDNUFGYOBWDQ-UHFFFAOYSA-N
Formula:	C19H37NO
SMILES:	CCCCCCN(CCCCCC)C(=O)C=C(C)C
Mol. weight [g/mol]:	295.50

Physical Properties

Property code	Value	Unit	Source
gf	162.63	kJ/mol	Joback Method
hf	-373.11	kJ/mol	Joback Method
hfus	48.48	kJ/mol	Joback Method
hvap	66.72	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.722		Crippen Method
mcvol	285.820	ml/mol	McGowan Method
pc	1169.62	kPa	Joback Method
rinsol	2099.00		NIST Webbook
tb	704.47	K	Joback Method
tc	877.89	K	Joback Method
tf	367.25	K	Joback Method
vc	1.105	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.07	J/mol×K	704.47	Joback Method
cpg	855.36	J/mol×K	733.37	Joback Method
cpg	873.74	J/mol×K	762.28	Joback Method
cpg	891.25	J/mol×K	791.18	Joback Method
cpg	907.93	J/mol×K	820.09	Joback Method
cpg	923.82	J/mol×K	848.99	Joback Method
cpg	938.98	J/mol×K	877.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U308240&Units=SI

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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