

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

Inchi:	InChI=1S/C25H49NO/c1-5-7-9-11-13-15-17-19-21-26(25(27)23-24(3)4)22-20-18-16-14-1
InchiKey:	WNDYPQJXPLTEQH-UHFFFAOYSA-N
Formula:	C25H49NO
SMILES:	CCCCCCCCCN(CCCCCCCCCC)C(=O)C=C(C)C
Mol. weight [g/mol]:	379.66

Physical Properties

Property code	Value	Unit	Source
gf	213.15	kJ/mol	Joback Method
hf	-496.95	kJ/mol	Joback Method
hfus	64.02	kJ/mol	Joback Method
hvap	80.07	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	8.063		Crippen Method
mcvol	370.360	ml/mol	McGowan Method
pc	816.33	kPa	Joback Method
rinsol	2695.00		NIST Webbook
tb	841.75	K	Joback Method
tc	1030.59	K	Joback Method
tf	434.87	K	Joback Method
vc	1.440	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1205.57	J/mol×K	841.75	Joback Method
cpg	1227.52	J/mol×K	873.22	Joback Method
cpg	1248.34	J/mol×K	904.70	Joback Method
cpg	1268.12	J/mol×K	936.17	Joback Method
cpg	1286.92	J/mol×K	967.64	Joback Method
cpg	1304.81	J/mol×K	999.12	Joback Method
cpg	1321.85	J/mol×K	1030.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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