

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

Inchi:	InChI=1S/C27H53NO/c1-5-7-9-11-13-15-17-19-21-23-28(27(29)25-26(3)4)24-22-20-18-1
InchiKey:	LDIPDNMMBQTOMM-UHFFFAOYSA-N
Formula:	C27H53NO
SMILES:	CCCCCCCCCCCN(CCCCCCCCCC)C(=O)C=C(C)C
Mol. weight [g/mol]:	407.72

Physical Properties

Property code	Value	Unit	Source
gf	229.99	kJ/mol	Joback Method
hf	-538.23	kJ/mol	Joback Method
hfus	69.20	kJ/mol	Joback Method
hvap	84.52	kJ/mol	Joback Method
log10ws	-9.32		Crippen Method
logp	8.843		Crippen Method
mvol	398.540	ml/mol	McGowan Method
pc	733.63	kPa	Joback Method
rinpol	2906.00		NIST Webbook
rinpol	2906.00		NIST Webbook
tb	887.51	K	Joback Method
tc	1087.87	K	Joback Method
tf	457.41	K	Joback Method
vc	1.552	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1334.85	J/mol×K	887.51	Joback Method
cpg	1358.13	J/mol×K	920.90	Joback Method
cpg	1380.16	J/mol×K	954.30	Joback Method
cpg	1401.05	J/mol×K	987.69	Joback Method
cpg	1420.88	J/mol×K	1021.09	Joback Method
cpg	1439.73	J/mol×K	1054.48	Joback Method
cpg	1457.69	J/mol×K	1087.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308245&Units=SI
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

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

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