Cyclobutanecarboxamide, N,N-diundecyl-

Inchi: InChI=1S/C27H53NO/c1-3-5-7-9-11-13-15-17-19-24-28(27(29)26-22-21-23-26)25-20-18-
InchiKey: YHGKEQBZOSZHDA-UHFFFAOYSA-N
Formula: C27H53NO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)C1CCC1
Mol. weight [g/mol]: 407.72

Physical Properties

Property code	Value	Unit	Source
gf	206.97	kJ/mol	Joback Method
hf	-579.02	kJ/mol	Joback Method
hfus	66.34	kJ/mol	Joback Method
hvap	84.57	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.677		Crippen Method
mcvol	391.980	ml/mol	McGowan Method
pc	774.18	kPa	Joback Method
rinpol	2919.00		NIST Webbook
rinpol	2919.00		NIST Webbook
tb	894.48	K	Joback Method
tc	1095.67	K	Joback Method
tf	490.87	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1351.17	J/mol×K	894.48	Joback Method
cpg	1374.67	J/mol×K	928.01	Joback Method
cpg	1396.87	J/mol×K	961.54	Joback Method
cpg	1417.86	J/mol×K	995.08	Joback Method
cpg	1437.75	J/mol×K	1028.61	Joback Method
cpg	1456.61	J/mol×K	1062.14	Joback Method
cpg	1474.54	J/mol×K	1095.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U308606&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
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
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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