Cyclobutanecarboxamide, N,N-dioctyl-

Inchi: InChI=1S/C21H41NO/c1-3-5-7-9-11-13-18-22(21(23)20-16-15-17-20)19-14-12-10-8-6-4-
InchiKey: URFQZOIRBJMQHE-UHFFFAOYSA-N
Formula: C21H41NO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)C1CCC1
Mol. weight [g/mol]: 323.56

Physical Properties

Property code	Value	Unit	Source
gf	156.45	kJ/mol	Joback Method
hf	-455.18	kJ/mol	Joback Method
hfus	50.80	kJ/mol	Joback Method
hvap	71.21	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.336		Crippen Method
mcvol	307.440	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	2312.00		NIST Webbook
tb	757.20	K	Joback Method
tc	936.86	K	Joback Method
tf	423.25	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.47	J/mol×K	757.20	Joback Method
cpg	990.34	J/mol×K	787.14	Joback Method
cpg	1010.15	J/mol×K	817.09	Joback Method
cpg	1028.95	J/mol×K	847.03	Joback Method
cpg	1046.80	J/mol×K	876.97	Joback Method
cpg	1063.76	J/mol×K	906.92	Joback Method
cpg	1079.86	J/mol×K	936.86	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=U308603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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