

Sarcosine, n-cyclopropylcarbonyl-, octyl ester

Inchi: InChI=1S/C15H27NO3/c1-3-4-5-6-7-8-11-19-14(17)12-16(2)15(18)13-9-10-13/h13H,3-12H
InchiKey: FHOIWWRQOYXQJQ-UHFFFAOYSA-N
Formula: C15H27NO3
SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)C1CC1
Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
hfus	40.15	kJ/mol	Joback Method
hvap	85.40	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.06		Cheméo Relay (1.0)
logp	2.758		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	581.48	K	Cheméo Relay (1.0)
tc	787.44	K	Cheméo Relay (1.0)
tf	296.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.87	J/mol×K	691.94	Joback Method
cpg	690.64	J/mol×K	722.44	Joback Method
cpg	706.53	J/mol×K	752.95	Joback Method
cpg	721.58	J/mol×K	783.45	Joback Method
cpg	735.82	J/mol×K	813.96	Joback Method
cpg	749.29	J/mol×K	844.46	Joback Method
cpg	762.03	J/mol×K	874.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321193&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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