

Sarcosine, N-hexanoyl-, pentadecyl ester

Inchi: InChI=1S/C24H47NO3/c1-4-6-8-9-10-11-12-13-14-15-16-17-19-21-28-24(27)22-25(3)23
InchiKey: IDKKLVGFWMTZRR-UHFFFAOYSA-N
Formula: C24H47NO3
SMILES: CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCCC
Mol. weight [g/mol]: 397.64

Physical Properties

Property code	Value	Unit	Source
hf	-943.16	kJ/mol	Cheméo Relay (1.0)
hfus	65.32	kJ/mol	Joback Method
hvap	118.14	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.90		Cheméo Relay (1.0)
logp	6.659		Crippen Method
mcvol	368.010	ml/mol	McGowan Method
pc	857.47	kPa	Joback Method
rinpol	2965.00		NIST Webbook
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tb	639.60	K	Cheméo Relay (1.0)
tc	832.79	K	Cheméo Relay (1.0)
tf	310.33	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1229.61	J/mol×K	891.12	Joback Method
cpg	1250.27	J/mol×K	924.61	Joback Method
cpg	1269.63	J/mol×K	958.10	Joback Method
cpg	1287.73	J/mol×K	991.60	Joback Method
cpg	1304.63	J/mol×K	1025.09	Joback Method
cpg	1320.38	J/mol×K	1058.58	Joback Method
cpg	1335.04	J/mol×K	1092.07	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U321130&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.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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

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