

Glycine, N-methyl-N-butoxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C22H43NO4/c1-4-6-8-9-10-11-12-13-14-15-16-17-19-26-21(24)20-23(3)22(25)
InchiKey: AIUNSNBXXHMCOG-UHFFFAOYSA-N
Formula: C22H43NO4
SMILES: CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)OCCCC
Mol. weight [g/mol]: 385.59

Physical Properties

Property code	Value	Unit	Source
af	1.1399		Cheméo Relay (1.0)
hf	-1066.77	kJ/mol	Cheméo Relay (1.0)
hfus	61.33	kJ/mol	Joback Method
hvap	116.73	kJ/mol	Cheméo Relay (1.0)
ie	9.03	eV	Cheméo Relay (1.0)
log10ws	-5.67		Cheméo Relay (1.0)
logp	6.099		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	952.60	kPa	Joback Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	632.56	K	Cheméo Relay (1.0)
tc	819.61	K	Cheméo Relay (1.0)
tf	286.68	K	Cheméo Relay (1.0)
vc	1.344	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.15	J/mol×K	867.78	Joback Method
cpg	1155.53	J/mol×K	900.23	Joback Method
cpg	1173.65	J/mol×K	932.68	Joback Method
cpg	1190.55	J/mol×K	965.13	Joback Method
cpg	1206.27	J/mol×K	997.58	Joback Method
cpg	1220.84	J/mol×K	1030.03	Joback Method
cpg	1234.29	J/mol×K	1062.48	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320658&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

af:	Acentric Factor
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
ie:	Ionization energy
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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