

«beta»-Alanine, N-caproyl-, heptyl ester

Inchi:	InChI=1S/C16H31NO3/c1-3-5-7-8-10-14-20-16(19)12-13-17-15(18)11-9-6-4-2/h3-14H2,1
InchiKey:	FOYMNYMFGOZPJU-UHFFFAOYSA-N
Formula:	C16H31NO3
SMILES:	CCCCCCCCOC(=O)CCNC(=O)CCCCC
Mol. weight [g/mol]:	285.42

Physical Properties

Property code	Value	Unit	Source
gf	-189.61	kJ/mol	Joback Method
hf	-677.48	kJ/mol	Joback Method
hfus	46.68	kJ/mol	Joback Method
hvap	73.55	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.587		Crippen Method
mcvol	255.290	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	2169.00		NIST Webbook
tb	745.81	K	Joback Method
tc	925.62	K	Joback Method
tf	444.83	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.84	J/mol×K	745.81	Joback Method
cpg	781.25	J/mol×K	775.78	Joback Method
cpg	796.80	J/mol×K	805.75	Joback Method
cpg	811.52	J/mol×K	835.72	Joback Method
cpg	825.42	J/mol×K	865.68	Joback Method
cpg	838.53	J/mol×K	895.65	Joback Method
cpg	850.85	J/mol×K	925.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321784&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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