

«beta»-Alanine, N-allyloxycarbonyl-, nonyl ester

Inchi:	InChI=1S/C16H29NO4/c1-3-5-6-7-8-9-10-14-20-15(18)11-12-17-16(19)21-13-4-2/h4H,2-
InchiKey:	RJBPUMPULHGYBT-UHFFFAOYSA-N
Formula:	C16H29NO4
SMILES:	C=CCOC(=O)NCCC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	299.41

Physical Properties

Property code	Value	Unit	Source
gf	-206.77	kJ/mol	Joback Method
hf	-684.27	kJ/mol	Joback Method
hfus	46.59	kJ/mol	Joback Method
hvap	75.29	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.583		Crippen Method
mvol	256.860	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
tb	764.91	K	Joback Method
tc	947.42	K	Joback Method
tf	465.30	K	Joback Method
vc	0.996	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.06	J/mol×K	764.91	Joback Method
cpg	784.72	J/mol×K	795.33	Joback Method
cpg	799.52	J/mol×K	825.75	Joback Method
cpg	813.46	J/mol×K	856.17	Joback Method
cpg	826.56	J/mol×K	886.59	Joback Method
cpg	838.83	J/mol×K	917.00	Joback Method
cpg	850.28	J/mol×K	947.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U321037&Units=SI

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

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