

L-Norvaline, N-propoxycarbonyl-, octadecyl ester

Inchi:	InChI=1S/C27H53NO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-31-26(29)23
InchiKey:	ZLJCCRORTBHPBD-UHFFFAOYSA-N
Formula:	C27H53NO4
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCCC
Mol. weight [g/mol]:	455.72

Physical Properties

Property code	Value	Unit	Source
hfus	72.84	kJ/mol	Joback Method
hvap	132.33	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.71		Cheméo Relay (1.0)
logp	8.096		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	731.65	kPa	Joback Method
tb	658.12	K	Cheméo Relay (1.0)
tc	857.68	K	Cheméo Relay (1.0)
tf	326.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.62	J/mol×K	1019.47	Joback Method
cpg	1497.09	J/mol×K	1060.83	Joback Method
cpg	1516.42	J/mol×K	1102.20	Joback Method
cpg	1533.69	J/mol×K	1143.56	Joback Method
cpg	1548.99	J/mol×K	1184.93	Joback Method
cpg	1562.39	J/mol×K	1226.29	Joback Method
cpg	1573.98	J/mol×K	1267.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320743&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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