

Sarcosine, N-(3-phenylpropionyl)-, pentyl ester

Inchi:	InChI=1S/C17H25NO3/c1-3-4-8-13-21-17(20)14-18(2)16(19)12-11-15-9-6-5-7-10-15/h5-
InchiKey:	CNYMWVBEMGMMKU-UHFFFAOYSA-N
Formula:	C17H25NO3
SMILES:	CCCCCOC(=O)CN(C)C(=O)CCc1ccccc1
Mol. weight [g/mol]:	291.39

Physical Properties

Property code	Value	Unit	Source
gf	-47.39	kJ/mol	Joback Method
hf	-447.53	kJ/mol	Joback Method
hfus	41.23	kJ/mol	Joback Method
hvap	73.66	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.811		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2306.00		NIST Webbook
rinpol	2306.00		NIST Webbook
tb	757.64	K	Joback Method
tc	956.43	K	Joback Method
tf	462.33	K	Joback Method
vc	0.927	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.56	J/molxK	757.64	Joback Method
cpg	733.54	J/molxK	790.77	Joback Method
cpg	748.50	J/molxK	823.90	Joback Method
cpg	762.47	J/molxK	857.03	Joback Method
cpg	775.49	J/molxK	890.16	Joback Method
cpg	787.61	J/molxK	923.30	Joback Method
cpg	798.87	J/molxK	956.43	Joback Method

Sources

Crippen Method:	https://www.chemeo.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=U321414&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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