

Sarcosine, n-(4-methylbenzoyl)-, isohexyl ester

Inchi:	InChI=1S/C17H25NO3/c1-13(2)6-5-11-21-16(19)12-18(4)17(20)15-9-7-14(3)8-10-15/h7-13,15-17,19-20,21
InchiKey:	JSONAPCYIXTJPS-UHFFFAOYSA-N
Formula:	C17H25NO3
SMILES:	<chem>Cc1ccc(C(=O)N(C)CC(=O)OCCCC(C)C)cc1</chem>
Mol. weight [g/mol]:	291.39

Physical Properties

Property code	Value	Unit	Source
hfus	37.32	kJ/mol	Joback Method
logp	3.046		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
rinpol	2266.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.44	J/mol×K	762.18	Joback Method
cpg	733.54	J/mol×K	795.90	Joback Method
cpg	748.59	J/mol×K	829.62	Joback Method
cpg	762.63	J/mol×K	863.34	Joback Method
cpg	775.70	J/mol×K	897.06	Joback Method
cpg	787.82	J/mol×K	930.78	Joback Method
cpg	799.04	J/mol×K	964.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321217&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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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