Sarcosine, N-(2-chlorobenzoyl)-, octyl ester

Inchi: InChI=1S/C18H26ClNO3/c1-3-4-5-6-7-10-13-23-17(21)14-20(2)18(22)15-11-8-9-12-16(1

InchiKey: CEZWRROFJUFQGM-UHFFFAOYSA-N

Formula: C18H26ClNO3

SMILES: CCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1Cl

Mol. weight [g/mol]: 339.86

Physical Properties

Property code	Value	Unit	Source
gf	-60.53	kJ/mol	Joback Method
hf	-495.38	kJ/mol	Joback Method
hfus	47.63	kJ/mol	Joback Method
hvap	80.93	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.316		Crippen Method
mcvol	271.950	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2536.00		NIST Webbook
tb	822.93	K	Joback Method
tc	1026.04	K	Joback Method
tf	516.04	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.68	J/mol×K	822.93	Joback Method
cpg	816.68	J/mol×K	856.78	Joback Method
cpg	830.65	J/mol×K	890.63	Joback Method
cpg	843.63	J/mol×K	924.49	Joback Method
cpg	855.66	J/mol×K	958.34	Joback Method
cpg	866.79	J/mol×K	992.19	Joback Method
cpg	877.06	J/mol×K	1026.04	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=U321208&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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