

Sarcosine, N-(4-nitrobenzoyl)-, isobutyl ester

Inchi:	InChI=1S/C14H18N2O5/c1-10(2)9-21-13(17)8-15(3)14(18)11-4-6-12(7-5-11)16(19)20/h4
InchiKey:	KTWBHNIUVDHBFS-UHFFFAOYSA-N
Formula:	C14H18N2O5
SMILES:	CC(C)COC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	294.30

Physical Properties

Property code	Value	Unit	Source
gf	-49.17	kJ/mol	Joback Method
hf	-413.12	kJ/mol	Joback Method
hfus	40.91	kJ/mol	Joback Method
hvap	83.84	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	1.866		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	2373.00		NIST Webbook
rinpol	2373.00		NIST Webbook
tb	845.38	K	Joback Method
tc	1073.50	K	Joback Method
tf	569.65	K	Joback Method
vc	0.836	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.54	J/mol×K	845.38	Joback Method
cpg	669.94	J/mol×K	883.40	Joback Method
cpg	681.25	J/mol×K	921.42	Joback Method
cpg	691.52	J/mol×K	959.44	Joback Method
cpg	700.79	J/mol×K	997.46	Joback Method
cpg	709.10	J/mol×K	1035.48	Joback Method
cpg	716.51	J/mol×K	1073.50	Joback Method

Sources

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=U321282&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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