Sarcosine, N-(4-methylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C18H27NO3/c1-4-5-6-7-8-13-22-17(20)14-19(3)18(21)16-11-9-15(2)10-12-16/h
InchiKey: LXWZXTIGPKMCKM-UHFFFAOYSA-N
Formula: C18H27NO3
SMILES: CCCCCCCOC(=O)CN(C)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
gf	-48.60	kJ/mol	Joback Method
hf	-479.64	kJ/mol	Joback Method
hfus	43.43	kJ/mol	Joback Method
hvap	76.55	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.581		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2413.00		NIST Webbook
tb	785.50	K	Joback Method
tc	984.22	K	Joback Method
tf	486.12	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.86	J/mol×K	785.50	Joback Method
cpg	789.98	J/mol×K	818.62	Joback Method
cpg	805.08	J/mol×K	851.74	Joback Method
cpg	819.18	J/mol×K	884.86	Joback Method
cpg	832.32	J/mol×K	917.98	Joback Method
cpg	844.54	J/mol×K	951.10	Joback Method
cpg	855.87	J/mol×K	984.22	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=U321219&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