Sarcosine, N-(4-trifluoromethylbenzoyl)-, octyl ester

Inchi: InChI=1S/C19H26F3NO3/c1-3-4-5-6-7-8-13-26-17(24)14-23(2)18(25)15-9-11-16(12-10-1

InchiKey: FZNICZUBYAITAP-UHFFFAOYSA-N

Formula: C19H26F3NO3

SMILES: CCCCCCCCOC(=O)CN(C)C(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 373.41

Physical Properties

Property code	Value	Unit	Source
gf	-621.77	kJ/mol	Joback Method
hf	-1097.36	kJ/mol	Joback Method
hfus	47.85	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.681		Crippen Method
mcvol	279.110	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
rinpol	2292.00		NIST Webbook
tb	802.96	K	Joback Method
tc	993.34	K	Joback Method
tf	501.58	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.60	J/mol×K	802.96	Joback Method
cpg	870.79	J/mol×K	834.69	Joback Method
cpg	884.99	J/mol×K	866.42	Joback Method
cpg	898.27	J/mol×K	898.15	Joback Method
cpg	910.68	J/mol×K	929.88	Joback Method
cpg	922.26	J/mol×K	961.61	Joback Method
cpg	933.06	J/mol×K	993.34	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=U321509&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