p-Decyl-«alpha»-«alpha»-«alpha»-trifluoroacetoph

Inchi: InChI=1S/C18H25F3O/c1-2-3-4-5-6-7-8-9-10-15-11-13-16(14-12-15)17(22)18(19,20)21/h
InchiKey: GJNWUVBDBVUZKP-UHFFFAOYSA-N
Formula: C18H25F3O
SMILES: CCCCCCCCCCc1ccc(C(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 314.39
CAS: 100444-41-5

Physical Properties

Property code	Value	Unit	Source
gf	-507.05	kJ/mol	Joback Method
hf	-899.45	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	61.60	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.115		Crippen Method
mcvol	247.600	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
tb	691.35	K	Joback Method
tc	873.41	K	Joback Method
tf	385.68	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.72	J/mol×K	691.35	Joback Method
cpg	723.34	J/mol×K	721.69	Joback Method
cpg	739.02	J/mol×K	752.04	Joback Method
cpg	753.81	J/mol×K	782.38	Joback Method
cpg	767.76	J/mol×K	812.72	Joback Method
cpg	780.92	J/mol×K	843.06	Joback Method
cpg	793.33	J/mol×K	873.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C100444415&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume