2,5-Di(trifluoromethyl)benzoic acid, decyl ester

Inchi: InChI=1S/C19H24F6O2/c1-2-3-4-5-6-7-8-9-12-27-17(26)15-13-14(18(20,21)22)10-11-16
InchiKey: YOQGEDMRMPFMJY-UHFFFAOYSA-N
Formula: C19H24F6O2
SMILES: CCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 398.38

Physical Properties

Property code	Value	Unit	Source
gf	-1194.85	kJ/mol	Joback Method
hf	-1660.86	kJ/mol	Joback Method
hfus	44.67	kJ/mol	Joback Method
hvap	63.15	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	7.022		Crippen Method
mcvol	272.870	ml/mol	McGowan Method
pc	1167.22	kPa	Joback Method
rinpol	1846.00		NIST Webbook
tb	736.21	K	Joback Method
tc	911.61	K	Joback Method
tf	435.89	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.50	J/mol×K	736.21	Joback Method
cpg	832.87	J/mol×K	765.44	Joback Method
cpg	847.35	J/mol×K	794.68	Joback Method
cpg	860.99	J/mol×K	823.91	Joback Method
cpg	873.82	J/mol×K	853.15	Joback Method
cpg	885.90	J/mol×K	882.38	Joback Method
cpg	897.28	J/mol×K	911.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338943&Units=SI
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

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