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

Inchi: InChI=1S/C26H38F6O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-34-24(33)22-20-21

InchiKey: PPYOIDNXHIXTDW-UHFFFAOYSA-N

Formula: C26H38F6O2

SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 496.57

Physical Properties

Property code	Value	Unit	Source
gf	-1135.91	kJ/mol	Joback Method
hf	-1805.34	kJ/mol	Joback Method
hfus	62.80	kJ/mol	Joback Method
hvap	78.73	kJ/mol	Joback Method
log10ws	-10.62		Crippen Method
logp	9.752		Crippen Method
mcvol	371.500	ml/mol	McGowan Method
pc	772.03	kPa	Joback Method
rinpol	2512.00		NIST Webbook
tb	896.37	K	Joback Method
tc	1099.18	K	Joback Method
tf	514.78	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1235.18	J/mol×K	896.37	Joback Method
cpg	1253.92	J/mol×K	930.17	Joback Method
cpg	1271.47	J/mol×K	963.97	Joback Method
cpg	1287.92	J/mol×K	997.78	Joback Method
cpg	1303.37	J/mol×K	1031.58	Joback Method
cpg	1317.90	J/mol×K	1065.38	Joback Method
cpg	1331.60	J/mol×K	1099.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338950&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

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