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

Inchi: InChI=1S/C20H26F6O2/c1-2-3-4-5-6-7-8-9-10-13-28-18(27)16-14-15(19(21,22)23)11-12

InchiKey: JVRQFSNUKYQKMA-UHFFFAOYSA-N

Formula: C20H26F6O2

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

Mol. weight [g/mol]: 412.41

Physical Properties

Property code	Value	Unit	Source
gf	-1186.43	kJ/mol	Joback Method
hf	-1681.50	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	65.38	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.412		Crippen Method
mcvol	286.960	ml/mol	McGowan Method
pc	1094.27	kPa	Joback Method
rinpol	1938.00		NIST Webbook
tb	759.09	K	Joback Method
tc	936.15	K	Joback Method
tf	447.16	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.67	J/mol×K	759.09	Joback Method
cpg	890.42	J/mol×K	788.60	Joback Method
cpg	905.26	J/mol×K	818.11	Joback Method
cpg	919.23	J/mol×K	847.62	Joback Method
cpg	932.38	J/mol×K	877.13	Joback Method
cpg	944.77	J/mol×K	906.64	Joback Method
cpg	956.43	J/mol×K	936.15	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=U338944&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

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