

2,5-Di(trifluoromethyl)benzoic acid, 3-tridecyl ester

Inchi:	InChI=1S/C22H30F6O2/c1-3-5-6-7-8-9-10-11-12-17(4-2)30-20(29)18-15-16(21(23,24)25
InchiKey:	NGXSLOKQJYFRCS-UHFFFAOYSA-N
Formula:	C22H30F6O2
SMILES:	CCCCCCCCCCC(CC)OC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]:	440.46

Physical Properties

Property code	Value	Unit	Source
gf	-1172.03	kJ/mol	Joback Method
hf	-1728.06	kJ/mol	Joback Method
hfus	48.91	kJ/mol	Joback Method
hvap	69.44	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	8.190		Crippen Method
mcvol	315.140	ml/mol	McGowan Method
pc	972.30	kPa	Joback Method
rinpola	2039.00		NIST Webbook
rinpola	2039.00		NIST Webbook
tb	804.41	K	Joback Method
tc	987.45	K	Joback Method
tf	454.70	K	Joback Method
vc	1.264	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.24	J/molxK	804.41	Joback Method
cpg	1008.88	J/molxK	834.92	Joback Method
cpg	1024.53	J/molxK	865.42	Joback Method
cpg	1039.24	J/molxK	895.93	Joback Method
cpg	1053.07	J/molxK	926.44	Joback Method
cpg	1066.07	J/molxK	956.94	Joback Method
cpg	1078.31	J/molxK	987.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U338701&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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