

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

Inchi:	InChI=1S/C23H32F6O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-31-21(30)19-17-18(22(24,25
InchiKey:	DLHDVUUBMKJPNF-UHFFFAOYSA-N
Formula:	C23H32F6O2
SMILES:	CCCCCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]:	454.49

Physical Properties

Property code	Value	Unit	Source
gf	-1161.17	kJ/mol	Joback Method
hf	-1743.42	kJ/mol	Joback Method
hfus	55.03	kJ/mol	Joback Method
hvap	72.05	kJ/mol	Joback Method
log10ws	-9.36		Crippen Method
logp	8.582		Crippen Method
mvol	329.230	ml/mol	McGowan Method
pc	912.18	kPa	Joback Method
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
tb	827.73	K	Joback Method
tc	1013.89	K	Joback Method
tf	480.97	K	Joback Method
vc	1.325	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1051.52	J/molxK	827.73	Joback Method
cpg	1068.56	J/molxK	858.76	Joback Method
cpg	1084.59	J/molxK	889.78	Joback Method
cpg	1099.65	J/molxK	920.81	Joback Method
cpg	1113.82	J/molxK	951.84	Joback Method
cpg	1127.16	J/molxK	982.86	Joback Method
cpg	1139.73	J/molxK	1013.89	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=U338947&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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