

2-Fluoro-5-trifluoromethylbenzoic acid, 4-tetradecyl ester

Inchi:	InChI=1S/C22H32F4O2/c1-3-5-6-7-8-9-10-11-13-18(12-4-2)28-21(27)19-16-17(22(24,25
InchiKey:	QHTAMVAYVIGRPG-UHFFFAOYSA-N
Formula:	C22H32F4O2
SMILES:	CCCCCCCCCCC(CCC)OC(=O)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]:	404.48

Physical Properties

Property code	Value	Unit	Source
gf	-785.25	kJ/mol	Joback Method
hf	-1327.09	kJ/mol	Joback Method
hfus	50.17	kJ/mol	Joback Method
hvap	72.37	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.701		Crippen Method
mcvol	311.600	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2171.00		NIST Webbook
rinpol	2171.00		NIST Webbook
tb	809.10	K	Joback Method
tc	994.47	K	Joback Method
tf	451.10	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.20	J/molxK	809.10	Joback Method
cpg	993.46	J/molxK	839.99	Joback Method
cpg	1009.71	J/molxK	870.89	Joback Method
cpg	1024.97	J/molxK	901.78	Joback Method
cpg	1039.30	J/molxK	932.68	Joback Method
cpg	1052.75	J/molxK	963.57	Joback Method
cpg	1065.36	J/molxK	994.47	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=U338629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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