

2,4,5-Trifluoro-3-methoxybenzoic acid, 3-tetradecyl ester

Inchi:	InChI=1S/C22H33F3O3/c1-4-6-7-8-9-10-11-12-13-14-16(5-2)28-22(26)17-15-18(23)20(2
InchiKey:	CUYCWLKQACBPC-UHFFFAOYSA-N
Formula:	C22H33F3O3
SMILES:	CCCCCCCCCCCC(CC)OC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]:	402.49

Physical Properties

Property code	Value	Unit	Source
gf	-717.54	kJ/mol	Joback Method
hf	-1277.39	kJ/mol	Joback Method
hfus	54.91	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	6.969		Crippen Method
mcvol	315.700	ml/mol	McGowan Method
pc	1003.35	kPa	Joback Method
rinpola	2432.00		NIST Webbook
rinpola	2432.00		NIST Webbook
tb	845.44	K	Joback Method
tc	1036.30	K	Joback Method
tf	495.36	K	Joback Method
vc	1.250	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.18	J/molxK	845.44	Joback Method
cpg	1015.38	J/molxK	877.25	Joback Method
cpg	1031.47	J/molxK	909.06	Joback Method
cpg	1046.45	J/molxK	940.87	Joback Method
cpg	1060.34	J/molxK	972.68	Joback Method
cpg	1073.15	J/molxK	1004.49	Joback Method
cpg	1084.91	J/molxK	1036.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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