

2-Fluoro-5-trifluoromethylbenzoic acid, heptyl ester

Inchi:	InChI=1S/C15H18F4O2/c1-2-3-4-5-6-9-21-14(20)12-10-11(15(17,18)19)7-8-13(12)16/h7
InchiKey:	YTBSWIJQERHZAT-UHFFFAOYSA-N
Formula:	C15H18F4O2
SMILES:	CCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]:	306.30

Physical Properties

Property code	Value	Unit	Source
gf	-841.75	kJ/mol	Joback Method
hf	-1177.33	kJ/mol	Joback Method
hfus	35.56	kJ/mol	Joback Method
hvap	57.18	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.972		Crippen Method
mcvol	212.970	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	649.38	K	Joback Method
tc	828.47	K	Joback Method
tf	387.21	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.55	J/molxK	649.38	Joback Method
cpg	594.98	J/molxK	679.23	Joback Method
cpg	608.62	J/molxK	709.08	Joback Method
cpg	621.50	J/molxK	738.93	Joback Method
cpg	633.64	J/molxK	768.78	Joback Method
cpg	645.08	J/molxK	798.62	Joback Method
cpg	655.84	J/molxK	828.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338961&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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