

# 4-Fluoro-3-trifluoromethylbenzoic acid, isoheptyl ester

<b>Inchi:</b>	InChI=1S/C14H16F4O2/c1-9(2)4-3-7-20-13(19)10-5-6-12(15)11(8-10)14(16,17)18/h5-6,8
<b>InchiKey:</b>	BOCVFRSIBOHIQE-UHFFFAOYSA-N
<b>Formula:</b>	C14H16F4O2
<b>SMILES:</b>	CC(C)CCCOC(=O)c1ccc(F)c(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	292.27

## Physical Properties

Property code	Value	Unit	Source
gf	-852.61	kJ/mol	Joback Method
hf	-1161.97	kJ/mol	Joback Method
hfus	29.45	kJ/mol	Joback Method
hvap	54.56	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.438		Crippen Method
mvol	198.880	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
tb	626.06	K	Joback Method
tc	809.25	K	Joback Method
tf	360.94	K	Joback Method
vc	0.790	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.19	J/mol×K	626.06	Joback Method
cpg	543.41	J/mol×K	656.59	Joback Method
cpg	556.84	J/mol×K	687.12	Joback Method
cpg	569.49	J/mol×K	717.66	Joback Method
cpg	581.39	J/mol×K	748.19	Joback Method
cpg	592.58	J/mol×K	778.72	Joback Method
cpg	603.08	J/mol×K	809.25	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U338917&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338917&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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