6-Fluoro-2-trifluoromethylbenzoic acid, heptyl ester

Inchi: InChI=1S/C15H18F4O2/c1-2-3-4-5-6-10-21-14(20)13-11(15(17,18)19)8-7-9-12(13)16/h7-

InchiKey: DDSRSQCEKWEPCD-UHFFFAOYSA-N

Formula: C15H18F4O2

SMILES: CCCCCCCOC(=O)c1c(F)cccc1C(F)(F)F

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	1632.00		NIST Webbook
rinpol	1632.00		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/mol×K	649.38	Joback Method
cpg	594.98	J/mol×K	679.23	Joback Method
cpg	608.62	J/mol×K	709.08	Joback Method
cpg	621.50	J/mol×K	738.93	Joback Method
cpg	633.64	J/mol×K	768.78	Joback Method
cpg	645.08	J/mol×K	798.62	Joback Method
cpg	655.84	J/mol×K	828.47	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=U338981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume