6-Fluoro-2-trifluoromethylbenzoic acid, dodecyl ester

Inchi: InChI=1S/C20H28F4O2/c1-2-3-4-5-6-7-8-9-10-11-15-26-19(25)18-16(20(22,23)24)13-12

InchiKey: URUTUPLDWKNQAT-UHFFFAOYSA-N

Formula: C20H28F4O2

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

Mol. weight [g/mol]: 376.43

Physical Properties

Property code	Value	Unit	Source
gf	-799.65	kJ/mol	Joback Method
hf	-1280.53	kJ/mol	Joback Method
hfus	48.51	kJ/mol	Joback Method
hvap	68.31	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.922		Crippen Method
mcvol	283.420	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	763.78	K	Joback Method
tc	943.85	K	Joback Method
tf	443.56	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.75	J/mol×K	763.78	Joback Method
cpg	874.15	J/mol×K	793.79	Joback Method
cpg	889.63	J/mol×K	823.80	Joback Method
cpg	904.22	J/mol×K	853.81	Joback Method
cpg	917.96	J/mol×K	883.82	Joback Method
cpg	930.88	J/mol×K	913.84	Joback Method
cpg	943.03	J/mol×K	943.85	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=U338986&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