4-Fluoro-3-trifluoromethylbenzoic acid, 6-dodecyl ester

Inchi: InChI=1S/C20H28F4O2/c1-3-5-7-9-11-16(10-8-6-4-2)26-19(25)15-12-13-18(21)17(14-15
InchiKey: QLWWECTTYYLTFD-UHFFFAOYSA-N
Formula: C20H28F4O2
SMILES: CCCCCCC(CCCCC)OC(=O)c1ccc(F)c(C(F)(F)F)c1
Mol. weight [g/mol]: 376.43

Physical Properties

Property code	Value	Unit	Source
gf	-802.09	kJ/mol	Joback Method
hf	-1285.81	kJ/mol	Joback Method
hfus	44.99	kJ/mol	Joback Method
hvap	67.92	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.921		Crippen Method
mcvol	283.420	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	1952.00		NIST Webbook
rinpol	1952.00		NIST Webbook
tb	763.34	K	Joback Method
tc	944.85	K	Joback Method
tf	428.56	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.25	J/mol×K	763.34	Joback Method
cpg	874.80	J/mol×K	793.59	Joback Method
cpg	890.39	J/mol×K	823.84	Joback Method
cpg	905.08	J/mol×K	854.10	Joback Method
cpg	918.89	J/mol×K	884.35	Joback Method
cpg	931.87	J/mol×K	914.60	Joback Method
cpg	944.06	J/mol×K	944.85	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=U338676&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