2-Trifluoromethylbenzoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C16H13F3O2/c1-10-7-11(2)9-12(8-10)21-15(20)13-5-3-4-6-14(13)16(17,18)19

InchiKey: OHUUJJZOHADYAG-UHFFFAOYSA-N

Formula: C16H13F3O2

SMILES: Cc1cc(C)cc(OC(=O)c2ccccc2C(F)(F)F)c1

Mol. weight [g/mol]: 294.27

Physical Properties

Property code	Value	Unit	Source
gf	-535.74	kJ/mol	Joback Method
hf	-776.80	kJ/mol	Joback Method
hfus	28.72	kJ/mol	Joback Method
hvap	63.16	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.541		Crippen Method
mcvol	201.530	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1808.00		NIST Webbook
rinpol	1808.00		NIST Webbook
tb	704.65	K	Joback Method
tc	922.76	K	Joback Method
tf	436.83	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.50	J/mol×K	704.65	Joback Method
cpg	556.50	J/mol×K	741.00	Joback Method
cpg	569.44	J/mol×K	777.35	Joback Method
cpg	581.38	J/mol×K	813.71	Joback Method
cpg	592.37	J/mol×K	850.06	Joback Method
cpg	602.47	J/mol×K	886.41	Joback Method
cpg	611.72	J/mol×K	922.76	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=U307670&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