3-Methoxybenzoic acid, 2-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C16H13F3O3/c1-21-13-7-4-6-11(9-13)15(20)22-10-12-5-2-3-8-14(12)16(17,18)

InchiKey: XIQQOCPUWOYQOR-UHFFFAOYSA-N

Formula: C16H13F3O3

SMILES: COc1cccc(C(=O)OCc2ccccc2C(F)(F)F)c1

Mol. weight [g/mol]: 310.27

Physical Properties

Property code	Value	Unit	Source
gf	-631.11	kJ/mol	Joback Method
hf	-897.55	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	64.91	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.071		Crippen Method
mcvol	207.400	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	2002.00		NIST Webbook
rinpol	2002.00		NIST Webbook
tb	722.09	K	Joback Method
tc	937.12	K	Joback Method
tf	446.54	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.53	J/mol×K	722.09	Joback Method
cpg	583.27	J/mol×K	757.93	Joback Method
cpg	595.94	J/mol×K	793.77	Joback Method
cpg	607.60	J/mol×K	829.61	Joback Method
cpg	618.28	J/mol×K	865.45	Joback Method
cpg	628.02	J/mol×K	901.29	Joback Method
cpg	636.87	J/mol×K	937.12	Joback Method

Sources

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=U374931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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