

4-(Methylthio)benzoic acid, 2-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C16H13F3O2S/c1-22-13-8-6-11(7-9-13)15(20)21-10-12-4-2-3-5-14(12)16(17,18)
InchiKey: DKTXCMZBYCZSRY-UHFFFAOYSA-N
Formula: C16H13F3O2S
SMILES: CSc1ccc(C(=O)OCc2ccccc2C(F)(F)F)cc1
Mol. weight [g/mol]: 326.33

Physical Properties

Property code	Value	Unit	Source
gf	-492.99	kJ/mol	Joback Method
hf	-723.46	kJ/mol	Joback Method
hfus	33.24	kJ/mol	Joback Method
hvap	69.31	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.784		Crippen Method
mvol	217.880	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook
tb	768.45	K	Joback Method
tc	1000.06	K	Joback Method
tf	458.71	K	Joback Method
vc	0.837	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.99	J/mol×K	768.45	Joback Method
cpg	609.14	J/mol×K	807.05	Joback Method
cpg	621.12	J/mol×K	845.65	Joback Method
cpg	631.98	J/mol×K	884.25	Joback Method
cpg	641.78	J/mol×K	922.85	Joback Method
cpg	650.58	J/mol×K	961.46	Joback Method
cpg	658.45	J/mol×K	1000.06	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=U375069&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/120-738-9/4-Methylthio-benzoic-acid-2-trifluoromethyl-benzyl-ester.pdf>

Generated by Cheméo on 2024-04-29 12:00:06.981140887 +0000 UTC m=+16681255.901718203.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.