

3-Trifluoromethylbenzoic acid, 3-methylbut-2-enyl ester

Inchi:	InChI=1S/C13H13F3O2/c1-9(2)6-7-18-12(17)10-4-3-5-11(8-10)13(14,15)16/h3-6,8H,7H2
InchiKey:	ZSJCOZKAUPZFTL-UHFFFAOYSA-N
Formula:	C13H13F3O2
SMILES:	CC(C)=CCOC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	258.24

Physical Properties

Property code	Value	Unit	Source
gf	-582.48	kJ/mol	Joback Method
hf	-821.04	kJ/mol	Joback Method
hfus	26.58	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.828		Crippen Method
mcvol	178.720	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1421.00		NIST Webbook
rinpol	1421.00		NIST Webbook
tb	603.41	K	Joback Method
tc	802.42	K	Joback Method
tf	332.52	K	Joback Method
vc	0.704	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.07	J/mol×K	603.41	Joback Method
cpg	463.97	J/mol×K	636.58	Joback Method
cpg	476.97	J/mol×K	669.75	Joback Method
cpg	489.12	J/mol×K	702.92	Joback Method
cpg	500.47	J/mol×K	736.09	Joback Method
cpg	511.06	J/mol×K	769.25	Joback Method
cpg	520.95	J/mol×K	802.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	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/53-241-5/3-Trifluoromethylbenzoic-acid-3-methylbut-2-enyl-ester.pdf>

Generated by Cheméo on 2024-04-19 20:43:07.439071547 +0000 UTC m=+15848636.359648862.

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