4-(Trifluoromethyl)benzoic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C13H13F3O2/c1-9(2)7-8-18-12(17)10-3-5-11(6-4-10)13(14,15)16/h3-7H,8H2,1

InchiKey: YKNOOVRCQWZGKB-UHFFFAOYSA-N

Formula: C13H13F3O2

SMILES: CC(C)=CCOC(=O)c1ccc(C(F)(F)F)cc1

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	1430.00		NIST Webbook
rinpol	1430.00		NIST Webbook
tb	603.41	K	Joback Method
tc	802.42	K	Joback Method
tf	332.52	K	Joback Method
vc	0.704	m3/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=U299439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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

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