2-Trifluoromethylbenzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C13H7F11O2/c14-9(15)11(18,19)13(23,24)10(16,17)5-26-8(25)6-3-1-2-4-7(6)1

InchiKey: VPUHCVJRBSAKGV-UHFFFAOYSA-N

Formula: C13H7F11O2

SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 404.18

Physical Properties

Property code	Value	Unit	Source
gf	-2206.55	kJ/mol	Joback Method
hf	-2528.88	kJ/mol	Joback Method
hfus	26.57	kJ/mol	Joback Method
hvap	42.07	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.033		Crippen Method
mcvol	197.180	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
tb	583.40	K	Joback Method
tc	744.47	K	Joback Method
tf	348.54	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.79	J/mol×K	583.40	Joback Method
cpg	557.84	J/mol×K	610.24	Joback Method
cpg	569.03	J/mol×K	637.09	Joback Method
cpg	579.39	J/mol×K	663.93	Joback Method
cpg	588.98	J/mol×K	690.78	Joback Method
cpg	597.86	J/mol×K	717.62	Joback Method
cpg	606.06	J/mol×K	744.47	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=U355150&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