Glutaric acid, 1,1,1-trifluoroprop-2-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C11H12F8O4/c1-6(10(14,15)16)23-8(21)4-2-3-7(20)22-5-9(12,13)11(17,18)19/

InchiKey: HUVRSTPXFYGASN-UHFFFAOYSA-N

Formula: C11H12F8O4

SMILES: CC(OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 360.20

Physical Properties

Property code	Value	Unit	Source
gf	-1978.50	kJ/mol	Joback Method
hf	-2360.38	kJ/mol	Joback Method
hfus	28.70	kJ/mol	Joback Method
hvap	47.58	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.391		Crippen Method
mcvol	194.890	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
tb	587.69	K	Joback Method
tc	742.15	K	Joback Method
tf	355.03	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.02	J/mol×K	587.69	Joback Method
cpg	551.81	J/mol×K	613.43	Joback Method
cpg	562.93	J/mol×K	639.18	Joback Method
cpg	573.41	J/mol×K	664.92	Joback Method
cpg	583.28	J/mol×K	690.66	Joback Method
cpg	592.56	J/mol×K	716.41	Joback Method
cpg	601.28	J/mol×K	742.15	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=U393663&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