Glutaric acid, 2,2-dichloroethyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C10H13Cl2F3O4/c1-6(10(13,14)15)19-9(17)4-2-3-8(16)18-5-7(11)12/h6-7H,2-5

InchiKey: AHTUOJCASOQEFL-UHFFFAOYSA-N

Formula: C10H13Cl2F3O4

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

Mol. weight [g/mol]: 325.11

Physical Properties

Property code	Value	Unit	Source
gf	-1044.85	kJ/mol	Joback Method
hf	-1378.45	kJ/mol	Joback Method
hfus	30.40	kJ/mol	Joback Method
hvap	60.41	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.998		Crippen Method
mcvol	196.430	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	1509.00		NIST Webbook
rinpol	1509.00		NIST Webbook
tb	649.34	K	Joback Method
tc	831.49	K	Joback Method
tf	380.81	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.26	J/mol×K	649.34	Joback Method
cpg	509.45	J/mol×K	679.70	Joback Method
cpg	519.99	J/mol×K	710.06	Joback Method
cpg	529.90	J/mol×K	740.42	Joback Method
cpg	539.17	J/mol×K	770.77	Joback Method
cpg	547.84	J/mol×K	801.13	Joback Method
cpg	555.92	J/mol×K	831.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393653&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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