Glutaric acid, 2,2-dichloroethyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C10H11Cl2F5O4/c11-6(12)4-20-7(18)2-1-3-8(19)21-5-9(13,14)10(15,16)17/h6

InchiKey: GXRUUNKQADVWNU-UHFFFAOYSA-N

Formula: C10H11Cl2F5O4

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

Mol. weight [g/mol]: 361.09

Physical Properties

Property code	Value	Unit	Source
gf	-1429.19	kJ/mol	Joback Method
hf	-1774.14	kJ/mol	Joback Method
hfus	32.67	kJ/mol	Joback Method
hvap	57.87	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.244		Crippen Method
mcvol	199.970	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	1454.00		NIST Webbook
rinpol	1454.00		NIST Webbook
tb	645.09	K	Joback Method
tc	819.49	K	Joback Method
tf	399.41	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.22	J/mol×K	645.09	Joback Method
cpg	527.66	J/mol×K	674.16	Joback Method
cpg	537.44	J/mol×K	703.22	Joback Method
cpg	546.60	J/mol×K	732.29	Joback Method
cpg	555.14	J/mol×K	761.35	Joback Method
cpg	563.11	J/mol×K	790.42	Joback Method
cpg	570.52	J/mol×K	819.49	Joback Method

Sources

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=U393669&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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