Glutaric acid, 2,2-dichloroethyl 2-fluoroethyl ester

Inchi: InChI=1S/C9H13Cl2FO4/c10-7(11)6-16-9(14)3-1-2-8(13)15-5-4-12/h7H,1-6H2
InchiKey: NDCNKNGTFYIKRI-UHFFFAOYSA-N
Formula: C9H13Cl2FO4
SMILES: O=C(CCCC(=O)OCC(Cl)Cl)OCCF
Mol. weight [g/mol]: 275.10

Physical Properties

Property code	Value	Unit	Source
gf	-664.05	kJ/mol	Joback Method
hf	-951.56	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	61.50	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	2.016		Crippen Method
mcvol	178.800	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1666.00		NIST Webbook
rinpol	1666.00		NIST Webbook
tb	631.59	K	Joback Method
tc	817.82	K	Joback Method
tf	380.94	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.98	J/mol×K	631.59	Joback Method
cpg	439.89	J/mol×K	662.63	Joback Method
cpg	450.25	J/mol×K	693.67	Joback Method
cpg	460.06	J/mol×K	724.70	Joback Method
cpg	469.33	J/mol×K	755.74	Joback Method
cpg	478.04	J/mol×K	786.78	Joback Method
cpg	486.20	J/mol×K	817.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393708&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