Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C12H12Cl2F8O4/c13-6(14)4-25-7(23)2-1-3-8(24)26-5-10(17,18)12(21,22)11(1

InchiKey: CMYGQYVUHOSMLJ-UHFFFAOYSA-N

Formula: C12H12Cl2F8O4

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

Mol. weight [g/mol]: 443.12

Physical Properties

Property code	Value	Unit	Source
gf	-1996.38	kJ/mol	Joback Method
hf	-2417.78	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	58.19	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.218		Crippen Method
mcvol	233.460	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	1676.00		NIST Webbook
tb	684.99	K	Joback Method
tc	852.59	K	Joback Method
tf	411.14	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.04	J/mol×K	684.99	Joback Method
cpg	656.78	J/mol×K	712.92	Joback Method
cpg	666.81	J/mol×K	740.86	Joback Method
cpg	676.15	J/mol×K	768.79	Joback Method
cpg	684.84	J/mol×K	796.73	Joback Method
cpg	692.92	J/mol×K	824.66	Joback Method
cpg	700.43	J/mol×K	852.59	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=U393536&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