

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

Inchi:	InChI=1S/C10H9ClF8O3/c11-5(20)2-1-3-6(21)22-4-8(14,15)10(18,19)9(16,17)7(12)13/h7
InchiKey:	WVUIFJKMLNKOXS-UHFFFAOYSA-N
Formula:	C10H9ClF8O3
SMILES:	O=C(Cl)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]:	364.62

Physical Properties

Property code	Value	Unit	Source
gf	-1893.85	kJ/mol	Joback Method
hf	-2223.26	kJ/mol	Joback Method
hfus	29.11	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.636		Crippen Method
mvol	187.170	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rmpol	1370.00		NIST Webbook
tb	579.82	K	Joback Method
tc	738.61	K	Joback Method
tf	351.45	K	Joback Method
vc	0.779	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.31	J/molxK	579.82	Joback Method
cpg	505.00	J/molxK	606.28	Joback Method
cpg	515.00	J/molxK	632.75	Joback Method
cpg	524.35	J/molxK	659.21	Joback Method
cpg	533.09	J/molxK	685.68	Joback Method
cpg	541.24	J/molxK	712.14	Joback Method
cpg	548.84	J/molxK	738.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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

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