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

Inchi: InChI=1S/C11H11F9O4/c12-8(13)9(14,15)4-23-6(21)2-1-3-7(22)24-5-10(16,17)11(18,19)

InchiKey: ICHHOTZYWAIWRA-UHFFFAOYSA-N

Formula: C11H11F9O4

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

Mol. weight [g/mol]: 378.19

Physical Properties

Property code	Value	Unit	Source
gf	-2173.31	kJ/mol	Joback Method
hf	-2556.49	kJ/mol	Joback Method
hfus	31.78	kJ/mol	Joback Method
hvap	46.76	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.341		Crippen Method
mcvol	196.660	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook
tb	586.96	K	Joback Method
tc	736.79	K	Joback Method
tf	355.62	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.17	J/mol×K	586.96	Joback Method
cpg	559.58	J/mol×K	611.93	Joback Method
cpg	570.36	J/mol×K	636.90	Joback Method
cpg	580.53	J/mol×K	661.88	Joback Method
cpg	590.11	J/mol×K	686.85	Joback Method
cpg	599.13	J/mol×K	711.82	Joback Method
cpg	607.62	J/mol×K	736.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393664&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

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

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