Glutaric acid, 1,1,1-trifluoroprop-2-yl 8-chlorooctyl ester

Inchi: InChI=1S/C16H26ClF3O4/c1-13(16(18,19)20)24-15(22)10-8-9-14(21)23-12-7-5-3-2-4-6-1

InchiKey: FPMVLQWQZLNSLY-UHFFFAOYSA-N

Formula: C16H26ClF3O4

SMILES: CC(OC(=O)CCCC(=O)OCCCCCCCCCl)C(F)(F)F

Mol. weight [g/mol]: 374.82

Physical Properties

Property code	Value	Unit	Source
gf	-979.96	kJ/mol	Joback Method
hf	-1481.27	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	69.77	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.773		Crippen Method
mcvol	268.730	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	2043.00		NIST Webbook
rinpol	2043.00		NIST Webbook
tb	749.63	K	Joback Method
tc	925.75	K	Joback Method
tf	433.51	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.22	J/mol×K	749.63	Joback Method
cpg	805.03	J/mol×K	778.98	Joback Method
cpg	819.01	J/mol×K	808.34	Joback Method
cpg	832.17	J/mol×K	837.69	Joback Method
cpg	844.54	J/mol×K	867.05	Joback Method
cpg	856.15	J/mol×K	896.40	Joback Method
cpg	867.01	J/mol×K	925.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393455&Units=SI

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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