Glutaric acid, 8-chlorooctyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C19H24ClF3O4/c20-12-5-3-1-2-4-6-13-26-16(24)8-7-9-17(25)27-15-11-10-14(2

InchiKey: SCDLIKGDRXURBP-UHFFFAOYSA-N

Formula: C19H24ClF3O4

SMILES: O=C(CCCC(=O)Oc1ccc(F)c(F)c1F)OCCCCCCCCCCl

Mol. weight [g/mol]: 408.84

Physical Properties

Property code	Value	Unit	Source
gf	-871.58	kJ/mol	Joback Method
hf	-1327.04	kJ/mol	Joback Method
hfus	56.85	kJ/mol	Joback Method
hvap	82.40	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.302		Crippen Method
mcvol	287.240	ml/mol	McGowan Method
pc	1243.33	kPa	Joback Method
rinpol	2624.00		NIST Webbook
tb	863.56	K	Joback Method
tc	1060.18	K	Joback Method
tf	543.88	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.46	J/mol×K	863.56	Joback Method
cpg	880.07	J/mol×K	896.33	Joback Method
cpg	892.66	J/mol×K	929.10	Joback Method
cpg	904.23	J/mol×K	961.87	Joback Method
cpg	914.80	J/mol×K	994.64	Joback Method
cpg	924.38	J/mol×K	1027.41	Joback Method
cpg	932.99	J/mol×K	1060.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393646&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