Glutaric acid, cyclohexylmethyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C18H21F3O4/c19-13-9-10-14(18(21)17(13)20)25-16(23)8-4-7-15(22)24-11-12-5-2-1-3-6-12/h9-10,12H,1-8,11H2

InchiKey: YFEPFUQRTLJWOB-UHFFFAOYSA-N

Formula: C18H21F3O4

SMILES: O=C(CCCC(=O)Oc1ccc(F)c(F)c1F)OCC1CCCCC1

Mol. weight [g/mol]: 358.35

Physical Properties

Property code	Value	Unit	Source
gf	-843.62	kJ/mol	Joback Method
hf	-1236.34	kJ/mol	Joback Method
hfus	41.90	kJ/mol	Joback Method
hvap	76.21	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.303		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	822.80	K	Joback Method
tc	1028.02	K	Joback Method
tf	510.07	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.70	J/mol×K	822.80	Joback Method
cpg	791.75	J/mol×K	857.00	Joback Method
cpg	805.59	J/mol×K	891.21	Joback Method
cpg	818.22	J/mol×K	925.41	Joback Method
cpg	829.66	J/mol×K	959.62	Joback Method
cpg	839.92	J/mol×K	993.82	Joback Method
cpg	849.00	J/mol×K	1028.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393641&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