Glutaric acid, hexyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C19H25F3O5/c1-2-3-4-5-13-25-17(23)7-6-8-18(24)26-14-15-9-11-16(12-10-15
InchiKey: GWJCDDDCJWAKQS-UHFFFAOYSA-N
Formula: C19H25F3O5
SMILES: CCCCCCOC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 390.39

Physical Properties

Property code	Value	Unit	Source
gf	-942.55	kJ/mol	Joback Method
hf	-1429.33	kJ/mol	Joback Method
hfus	47.21	kJ/mol	Joback Method
hvap	77.80	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.922		Crippen Method
mcvol	280.870	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
tb	835.36	K	Joback Method
tc	1028.98	K	Joback Method
tf	513.57	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.48	J/mol×K	835.36	Joback Method
cpg	885.89	J/mol×K	867.63	Joback Method
cpg	899.25	J/mol×K	899.90	Joback Method
cpg	911.57	J/mol×K	932.17	Joback Method
cpg	922.88	J/mol×K	964.44	Joback Method
cpg	933.21	J/mol×K	996.71	Joback Method
cpg	942.58	J/mol×K	1028.98	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=U377338&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