Glutaric acid, di(4-(trifluoromethoxy)benzyl) ester

Inchi: InChI=1S/C21H18F6O6/c22-20(23,24)32-16-8-4-14(5-9-16)12-30-18(28)2-1-3-19(29)31-

InchiKey: FTWLSFQXVDGWCR-UHFFFAOYSA-N

Formula: C21H18F6O6

SMILES: O=C(CCCC(=O)OCc1ccc(OC(F)(F)F)cc1)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 480.35

Physical Properties

Property code	Value	Unit	Source
gf	-1509.52	kJ/mol	Joback Method
hf	-1974.85	kJ/mol	Joback Method
hfus	49.05	kJ/mol	Joback Method
hvap	83.85	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.441		Crippen Method
mcvol	296.470	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
tb	929.78	K	Joback Method
tc	1140.78	K	Joback Method
tf	601.47	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.34	J/mol×K	929.78	Joback Method
cpg	947.29	J/mol×K	964.95	Joback Method
cpg	957.03	J/mol×K	1000.11	Joback Method
cpg	965.63	J/mol×K	1035.28	Joback Method
cpg	973.11	J/mol×K	1070.44	Joback Method
cpg	979.53	J/mol×K	1105.61	Joback Method
cpg	984.93	J/mol×K	1140.78	Joback Method

Sources

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=U377350&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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