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

Inchi: InChI=1S/C21H18F6O4/c22-20(23,24)16-8-4-14(5-9-16)12-30-18(28)2-1-3-19(29)31-13-

InchiKey: AUUSXXRTGNQAQF-UHFFFAOYSA-N

Formula: C21H18F6O4

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

Mol. weight [g/mol]: 448.36

Physical Properties

Property code	Value	Unit	Source
gf	-1299.52	kJ/mol	Joback Method
hf	-1710.41	kJ/mol	Joback Method
hfus	46.68	kJ/mol	Joback Method
hvap	79.03	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	5.681		Crippen Method
mcvol	284.730	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	884.94	K	Joback Method
tc	1091.05	K	Joback Method
tf	557.01	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.51	J/mol×K	884.94	Joback Method
cpg	895.57	J/mol×K	919.29	Joback Method
cpg	906.60	J/mol×K	953.64	Joback Method
cpg	916.69	J/mol×K	987.99	Joback Method
cpg	925.90	J/mol×K	1022.35	Joback Method
cpg	934.31	J/mol×K	1056.70	Joback Method
cpg	941.98	J/mol×K	1091.05	Joback Method

Sources

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=U377587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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