Glutaric acid, 2-methylhex-3-yl 4-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C20H27F3O4/c1-4-6-17(14(2)3)27-19(25)8-5-7-18(24)26-13-15-9-11-16(12-10

InchiKey: WQPFIAYWZBXOOG-UHFFFAOYSA-N

Formula: C20H27F3O4

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

Mol. weight [g/mol]: 388.42

Physical Properties

Property code	Value	Unit	Source
gf	-834.01	kJ/mol	Joback Method
hf	-1328.31	kJ/mol	Joback Method
hfus	41.56	kJ/mol	Joback Method
hvap	76.84	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.287		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	834.94	K	Joback Method
tc	1030.90	K	Joback Method
tf	472.61	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.96	J/mol×K	834.94	Joback Method
cpg	917.22	J/mol×K	867.60	Joback Method
cpg	931.40	J/mol×K	900.26	Joback Method
cpg	944.52	J/mol×K	932.92	Joback Method
cpg	956.65	J/mol×K	965.58	Joback Method
cpg	967.80	J/mol×K	998.24	Joback Method
cpg	978.03	J/mol×K	1030.90	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=U377581&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