Glutaric acid, heptyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C20H27F3O5/c1-2-3-4-5-6-14-26-18(24)8-7-9-19(25)27-15-16-10-12-17(13-11

InchiKey: XTMKQMQRCLXZBD-UHFFFAOYSA-N

Formula: C20H27F3O5

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

Mol. weight [g/mol]: 404.42

Physical Properties

Property code	Value	Unit	Source
gf	-934.13	kJ/mol	Joback Method
hf	-1449.97	kJ/mol	Joback Method
hfus	49.80	kJ/mol	Joback Method
hvap	80.03	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.312		Crippen Method
mcvol	294.960	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2374.00		NIST Webbook
tb	858.24	K	Joback Method
tc	1054.16	K	Joback Method
tf	524.84	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.89	J/mol×K	858.24	Joback Method
cpg	944.59	J/mol×K	890.89	Joback Method
cpg	958.18	J/mol×K	923.55	Joback Method
cpg	970.68	J/mol×K	956.20	Joback Method
cpg	982.13	J/mol×K	988.86	Joback Method
cpg	992.55	J/mol×K	1021.51	Joback Method
cpg	1001.97	J/mol×K	1054.16	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=U377339&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