Glutaric acid, propyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C16H19F3O5/c1-2-10-22-14(20)4-3-5-15(21)23-11-12-6-8-13(9-7-12)24-16(17
InchiKey: GTDNLVLXEYJJMM-UHFFFAOYSA-N
Formula: C16H19F3O5
SMILES: CCCOC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 348.31

Physical Properties

Property code	Value	Unit	Source
gf	-967.81	kJ/mol	Joback Method
hf	-1367.41	kJ/mol	Joback Method
hfus	39.44	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.752		Crippen Method
mcvol	238.600	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	1981.00		NIST Webbook
tb	766.72	K	Joback Method
tc	957.65	K	Joback Method
tf	479.76	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.26	J/mol×K	766.72	Joback Method
cpg	714.75	J/mol×K	798.54	Joback Method
cpg	727.32	J/mol×K	830.36	Joback Method
cpg	738.98	J/mol×K	862.19	Joback Method
cpg	749.75	J/mol×K	894.01	Joback Method
cpg	759.65	J/mol×K	925.83	Joback Method
cpg	768.70	J/mol×K	957.65	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=U377334&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