Glutaric acid, 1,1,1-trifluoroprop-2-yl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C16H19F3O5/c1-10-7-8-12(22-3)13(9-10)24-15(21)6-4-5-14(20)23-11(2)16(17

InchiKey: MWGSBTPJTVGLJR-UHFFFAOYSA-N

Formula: C16H19F3O5

SMILES: COc1ccc(C)cc1OC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 348.31

Physical Properties

Property code	Value	Unit	Source
gf	-979.88	kJ/mol	Joback Method
hf	-1384.16	kJ/mol	Joback Method
hfus	35.52	kJ/mol	Joback Method
hvap	71.40	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.573		Crippen Method
mcvol	238.600	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
tb	771.26	K	Joback Method
tc	965.20	K	Joback Method
tf	477.28	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.87	J/mol×K	771.26	Joback Method
cpg	714.42	J/mol×K	803.58	Joback Method
cpg	727.03	J/mol×K	835.91	Joback Method
cpg	738.71	J/mol×K	868.23	Joback Method
cpg	749.47	J/mol×K	900.56	Joback Method
cpg	759.32	J/mol×K	932.88	Joback Method
cpg	768.28	J/mol×K	965.20	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=U393918&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