Glutaric acid, 3-methylbut-2-en-1-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C16H17F3O4/c1-10(2)8-9-22-13(20)4-3-5-14(21)23-12-7-6-11(17)15(18)16(12

InchiKey: IXZFVCFAKHRGFF-UHFFFAOYSA-N

Formula: C16H17F3O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 330.30

Physical Properties

Property code	Value	Unit	Source
gf	-813.24	kJ/mol	Joback Method
hf	-1141.95	kJ/mol	Joback Method
hfus	43.78	kJ/mol	Joback Method
hvap	71.37	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.689		Crippen Method
mcvol	228.430	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	1991.00		NIST Webbook
rinpol	1991.00		NIST Webbook
tb	761.53	K	Joback Method
tc	954.45	K	Joback Method
tf	461.11	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.81	J/mol×K	761.53	Joback Method
cpg	657.80	J/mol×K	793.68	Joback Method
cpg	669.98	J/mol×K	825.84	Joback Method
cpg	681.37	J/mol×K	857.99	Joback Method
cpg	691.98	J/mol×K	890.14	Joback Method
cpg	701.82	J/mol×K	922.30	Joback Method
cpg	710.91	J/mol×K	954.45	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=U393637&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