Glutaric acid, propyl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C15H17F3O4/c1-2-8-21-13(19)4-3-5-14(20)22-9-10-11(16)6-7-12(17)15(10)18
InchiKey: DTXBSMBYUBXPCW-UHFFFAOYSA-N
Formula: C15H17F3O4
SMILES: CCCOC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 318.29

Physical Properties

Property code	Value	Unit	Source
gf	-893.33	kJ/mol	Joback Method
hf	-1228.74	kJ/mol	Joback Method
hfus	42.29	kJ/mol	Joback Method
hvap	69.11	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.271		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1944.00		NIST Webbook
rinpol	1944.00		NIST Webbook
tb	734.61	K	Joback Method
tc	921.00	K	Joback Method
tf	468.88	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.27	J/mol×K	734.61	Joback Method
cpg	628.26	J/mol×K	765.67	Joback Method
cpg	640.50	J/mol×K	796.74	Joback Method
cpg	651.97	J/mol×K	827.80	Joback Method
cpg	662.68	J/mol×K	858.87	Joback Method
cpg	672.63	J/mol×K	889.93	Joback Method
cpg	681.82	J/mol×K	921.00	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=U376894&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