Glutaric acid, 2,2,2-triluoroethyl octyl ester

Inchi: InChI=1S/C15H25F3O4/c1-2-3-4-5-6-7-11-21-13(19)9-8-10-14(20)22-12-15(16,17)18/h2-
InchiKey: CHQOAXJUTGFCFP-UHFFFAOYSA-N
Formula: C15H25F3O4
SMILES: CCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 326.35

Physical Properties

Property code	Value	Unit	Source
gf	-974.01	kJ/mol	Joback Method
hf	-1439.61	kJ/mol	Joback Method
hfus	42.01	kJ/mol	Joback Method
hvap	63.55	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.166		Crippen Method
mcvol	242.400	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook
tb	689.76	K	Joback Method
tc	857.37	K	Joback Method
tf	407.32	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.17	J/mol×K	689.76	Joback Method
cpg	718.18	J/mol×K	717.69	Joback Method
cpg	732.44	J/mol×K	745.63	Joback Method
cpg	745.98	J/mol×K	773.56	Joback Method
cpg	758.81	J/mol×K	801.50	Joback Method
cpg	770.94	J/mol×K	829.43	Joback Method
cpg	782.39	J/mol×K	857.37	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=U380515&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