Glutaric acid, butyl 2,2,2-triluoroethyl ester

Inchi: InChI=1S/C11H17F3O4/c1-2-3-7-17-9(15)5-4-6-10(16)18-8-11(12,13)14/h2-8H2,1H3
InchiKey: WFSRCSGNUTUBLG-UHFFFAOYSA-N
Formula: C11H17F3O4
SMILES: CCCCOC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 270.25

Physical Properties

Property code	Value	Unit	Source
gf	-1007.69	kJ/mol	Joback Method
hf	-1357.05	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	54.65	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.606		Crippen Method
mcvol	186.040	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	1311.00		NIST Webbook
rinpol	1311.00		NIST Webbook
tb	598.24	K	Joback Method
tc	764.99	K	Joback Method
tf	362.24	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.55	J/mol×K	598.24	Joback Method
cpg	505.39	J/mol×K	626.03	Joback Method
cpg	517.63	J/mol×K	653.82	Joback Method
cpg	529.29	J/mol×K	681.61	Joback Method
cpg	540.38	J/mol×K	709.41	Joback Method
cpg	550.90	J/mol×K	737.20	Joback Method
cpg	560.87	J/mol×K	764.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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