Glutaric acid, 1,1,1-trifluoroprop-2-yl decyl ester

Inchi: InChI=1S/C18H31F3O4/c1-3-4-5-6-7-8-9-10-14-24-16(22)12-11-13-17(23)25-15(2)18(19

InchiKey: VQRFELYDJZSMJK-UHFFFAOYSA-N

Formula: C18H31F3O4

SMILES: CCCCCCCCCCOC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 368.43

Physical Properties

Property code	Value	Unit	Source
gf	-951.19	kJ/mol	Joback Method
hf	-1506.81	kJ/mol	Joback Method
hfus	46.25	kJ/mol	Joback Method
hvap	69.84	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.335		Crippen Method
mcvol	284.670	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	1941.00		NIST Webbook
rinpol	1941.00		NIST Webbook
tb	757.96	K	Joback Method
tc	932.27	K	Joback Method
tf	426.13	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.33	J/mol×K	757.96	Joback Method
cpg	890.88	J/mol×K	787.01	Joback Method
cpg	906.53	J/mol×K	816.06	Joback Method
cpg	921.30	J/mol×K	845.12	Joback Method
cpg	935.22	J/mol×K	874.17	Joback Method
cpg	948.30	J/mol×K	903.22	Joback Method
cpg	960.58	J/mol×K	932.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391546&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