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

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

InchiKey: UTNZLXHROSNGSX-UHFFFAOYSA-N

Formula: C18H31F3O4

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

Mol. weight [g/mol]: 368.43

Physical Properties

Property code	Value	Unit	Source
gf	-953.63	kJ/mol	Joback Method
hf	-1512.09	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.333		Crippen Method
mcvol	284.670	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
rinpol	1831.00		NIST Webbook
rinpol	1831.00		NIST Webbook
tb	757.52	K	Joback Method
tc	932.82	K	Joback Method
tf	411.13	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.83	J/mol×K	757.52	Joback Method
cpg	891.48	J/mol×K	786.74	Joback Method
cpg	907.22	J/mol×K	815.95	Joback Method
cpg	922.06	J/mol×K	845.17	Joback Method
cpg	936.03	J/mol×K	874.39	Joback Method
cpg	949.16	J/mol×K	903.61	Joback Method
cpg	961.46	J/mol×K	932.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393502&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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