Glutaric acid, decyl 2,2,2-triluoroethyl ester

Inchi: InChI=1S/C17H29F3O4/c1-2-3-4-5-6-7-8-9-13-23-15(21)11-10-12-16(22)24-14-17(18,19
InchiKey: GGYUXSNBJHTZBV-UHFFFAOYSA-N
Formula: C17H29F3O4
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 354.40

Physical Properties

Property code	Value	Unit	Source
gf	-957.17	kJ/mol	Joback Method
hf	-1480.89	kJ/mol	Joback Method
hfus	47.19	kJ/mol	Joback Method
hvap	68.00	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.946		Crippen Method
mcvol	270.580	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	735.52	K	Joback Method
tc	906.41	K	Joback Method
tf	429.86	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.91	J/mol×K	735.52	Joback Method
cpg	831.88	J/mol×K	764.00	Joback Method
cpg	847.01	J/mol×K	792.48	Joback Method
cpg	861.34	J/mol×K	820.97	Joback Method
cpg	874.87	J/mol×K	849.45	Joback Method
cpg	887.63	J/mol×K	877.93	Joback Method
cpg	899.64	J/mol×K	906.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380517&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