Glutaric acid, dodecyl 2,2,2-triluoroethyl ester

Inchi: InChI=1S/C19H33F3O4/c1-2-3-4-5-6-7-8-9-10-11-15-25-17(23)13-12-14-18(24)26-16-19
InchiKey: MHUFPHWQGWVTLE-UHFFFAOYSA-N
Formula: C19H33F3O4
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 382.46

Physical Properties

Property code	Value	Unit	Source
gf	-940.33	kJ/mol	Joback Method
hf	-1522.17	kJ/mol	Joback Method
hfus	52.37	kJ/mol	Joback Method
hvap	72.45	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.726		Crippen Method
mcvol	298.760	ml/mol	McGowan Method
pc	1063.79	kPa	Joback Method
rinpol	2115.00		NIST Webbook
rinpol	2115.00		NIST Webbook
tb	781.28	K	Joback Method
tc	957.97	K	Joback Method
tf	452.40	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.72	J/mol×K	781.28	Joback Method
cpg	949.67	J/mol×K	810.73	Joback Method
cpg	965.68	J/mol×K	840.18	Joback Method
cpg	980.77	J/mol×K	869.62	Joback Method
cpg	994.97	J/mol×K	899.07	Joback Method
cpg	1008.31	J/mol×K	928.52	Joback Method
cpg	1020.82	J/mol×K	957.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380519&Units=SI

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