Glutaric acid, 2,2,3,3-tetrafluoropropyl tridecyl ester

Inchi: InChI=1S/C21H36F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-28-18(26)14-13-15-19(27)29-17
InchiKey: BNQNLZMGMUUGJR-UHFFFAOYSA-N
Formula: C21H36F4O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 428.50

Physical Properties

Property code	Value	Unit	Source
gf	-1120.74	kJ/mol	Joback Method
hf	-1764.84	kJ/mol	Joback Method
hfus	57.10	kJ/mol	Joback Method
hvap	75.70	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.454		Crippen Method
mcvol	328.710	ml/mol	McGowan Method
pc	921.06	kPa	Joback Method
rinpol	2338.00		NIST Webbook
rinpol	2338.00		NIST Webbook
tb	825.87	K	Joback Method
tc	1011.25	K	Joback Method
tf	460.53	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1060.84	J/mol×K	825.87	Joback Method
cpg	1078.76	J/mol×K	856.77	Joback Method
cpg	1095.57	J/mol×K	887.66	Joback Method
cpg	1111.33	J/mol×K	918.56	Joback Method
cpg	1126.07	J/mol×K	949.46	Joback Method
cpg	1139.82	J/mol×K	980.35	Joback Method
cpg	1152.62	J/mol×K	1011.25	Joback Method

Sources

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=U391625&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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