Glutaric acid, 2,2,3,3-tetrafluoropropyl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C20H30F4O4/c1-2-3-4-5-6-7-8-9-10-11-15-27-17(25)13-12-14-18(26)28-16-20

InchiKey: ABSDBGXAOOTARX-UHFFFAOYSA-N

Formula: C20H30F4O4

SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 410.44

Physical Properties

Property code	Value	Unit	Source
gf	-926.36	kJ/mol	Joback Method
hf	-1471.90	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	75.63	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.288		Crippen Method
mcvol	306.020	ml/mol	McGowan Method
pc	1082.78	kPa	Joback Method
rinpol	2281.00		NIST Webbook
rinpol	2281.00		NIST Webbook
tb	811.99	K	Joback Method
tc	996.21	K	Joback Method
tf	555.36	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.12	J/mol×K	811.99	Joback Method
cpg	967.27	J/mol×K	842.69	Joback Method
cpg	982.45	J/mol×K	873.40	Joback Method
cpg	996.68	J/mol×K	904.10	Joback Method
cpg	1010.00	J/mol×K	934.81	Joback Method
cpg	1022.42	J/mol×K	965.51	Joback Method
cpg	1033.98	J/mol×K	996.21	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=U393938&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