Glutaric acid, 2-(adamant-1-yl)ethyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C20H29F3O4/c1-13(20(21,22)23)27-18(25)4-2-3-17(24)26-6-5-19-10-14-7-15(

InchiKey: NDWCMKIKTVMUDZ-UHFFFAOYSA-N

Formula: C20H29F3O4

SMILES: CC(OC(=O)CCCC(=O)OCCC12CC3CC(CC(C3)C1)C2)C(F)(F)F

Mol. weight [g/mol]: 390.44

Physical Properties

Property code	Value	Unit	Source
gf	-777.40	kJ/mol	Joback Method
hf	-1340.95	kJ/mol	Joback Method
hfus	38.51	kJ/mol	Joback Method
hvap	72.74	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.800		Crippen Method
mcvol	280.270	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	823.78	K	Joback Method
tc	1022.90	K	Joback Method
tf	518.63	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.45	J/mol×K	823.78	Joback Method
cpg	967.35	J/mol×K	856.97	Joback Method
cpg	985.70	J/mol×K	890.15	Joback Method
cpg	1003.63	J/mol×K	923.34	Joback Method
cpg	1021.32	J/mol×K	956.53	Joback Method
cpg	1038.92	J/mol×K	989.72	Joback Method
cpg	1056.60	J/mol×K	1022.90	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=U405373&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