Glutaric acid, 2-(adamant-1-yl)ethyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C20H28F4O4/c21-18(22)20(23,24)12-28-17(26)3-1-2-16(25)27-5-4-19-9-13-6-14(10-19)8-15(7-13)11-19/h13-15,18H,1-12H2

InchiKey: UAZBIVUSIGHUFA-UHFFFAOYSA-N

Formula: C20H28F4O4

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

Mol. weight [g/mol]: 408.43

Physical Properties

Property code	Value	Unit	Source
gf	-972.21	kJ/mol	Joback Method
hf	-1537.06	kJ/mol	Joback Method
hfus	41.59	kJ/mol	Joback Method
hvap	71.92	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.750		Crippen Method
mcvol	282.040	ml/mol	McGowan Method
pc	1301.41	kPa	Joback Method
rinpol	2371.00		NIST Webbook
tb	823.05	K	Joback Method
tc	1018.01	K	Joback Method
tf	519.22	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.82	J/mol×K	823.05	Joback Method
cpg	974.23	J/mol×K	855.54	Joback Method
cpg	992.08	J/mol×K	888.04	Joback Method
cpg	1009.53	J/mol×K	920.53	Joback Method
cpg	1026.73	J/mol×K	953.02	Joback Method
cpg	1043.83	J/mol×K	985.52	Joback Method
cpg	1060.98	J/mol×K	1018.01	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=U405374&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