Glutaric acid, 1-(cyclohex-2-enyl)hex-3-yl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C20H31F3O4/c1-3-8-17(14-13-16-9-5-4-6-10-16)27-19(25)12-7-11-18(24)26-1

InchiKey: VILHNBUYVUTLEO-UHFFFAOYSA-N

Formula: C20H31F3O4

SMILES: CCCC(CCC1C=CCCC1)OC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 392.45

Physical Properties

Property code	Value	Unit	Source
gf	-882.38	kJ/mol	Joback Method
hf	-1441.27	kJ/mol	Joback Method
hfus	40.97	kJ/mol	Joback Method
hvap	74.62	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.499		Crippen Method
mcvol	297.690	ml/mol	McGowan Method
pc	1184.97	kPa	Joback Method
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
tb	821.99	K	Joback Method
tc	1014.50	K	Joback Method
tf	441.81	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.45	J/mol×K	821.99	Joback Method
cpg	979.73	J/mol×K	854.07	Joback Method
cpg	995.81	J/mol×K	886.16	Joback Method
cpg	1010.72	J/mol×K	918.24	Joback Method
cpg	1024.51	J/mol×K	950.33	Joback Method
cpg	1037.20	J/mol×K	982.41	Joback Method
cpg	1048.85	J/mol×K	1014.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405513&Units=SI
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

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