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

Inchi: InChI=1S/C20H30F4O4/c1-2-7-16(13-12-15-8-4-3-5-9-15)28-18(26)11-6-10-17(25)27-14
InchiKey: IVFVVYBDFIDZTQ-UHFFFAOYSA-N
Formula: C20H30F4O4
SMILES: CCCC(CCC1C=CCCC1)OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 410.44

Physical Properties

Property code	Value	Unit	Source
gf	-1077.19	kJ/mol	Joback Method
hf	-1637.38	kJ/mol	Joback Method
hfus	44.05	kJ/mol	Joback Method
hvap	73.81	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.449		Crippen Method
mcvol	299.460	ml/mol	McGowan Method
pc	1149.10	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	821.26	K	Joback Method
tc	1010.70	K	Joback Method
tf	442.40	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.84	J/mol×K	821.26	Joback Method
cpg	986.77	J/mol×K	852.83	Joback Method
cpg	1002.52	J/mol×K	884.41	Joback Method
cpg	1017.13	J/mol×K	915.98	Joback Method
cpg	1030.65	J/mol×K	947.55	Joback Method
cpg	1043.11	J/mol×K	979.12	Joback Method
cpg	1054.55	J/mol×K	1010.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405514&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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