Glutaric acid, (2-methylcyclohex-1-enyl)methyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C16H22F4O4/c1-11-5-2-3-6-12(11)9-23-13(21)7-4-8-14(22)24-10-16(19,20)15

InchiKey: NGSVOBXUWVVTJX-UHFFFAOYSA-N

Formula: C16H22F4O4

SMILES: CC1=C(COC(=O)CCCC(=O)OCC(F)(F)C(F)F)CCCC1

Mol. weight [g/mol]: 354.34

Physical Properties

Property code	Value	Unit	Source
gf	-1119.98	kJ/mol	Joback Method
hf	-1552.14	kJ/mol	Joback Method
hfus	35.36	kJ/mol	Joback Method
hvap	66.92	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.034		Crippen Method
mcvol	243.100	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	1871.00		NIST Webbook
rinpol	1871.00		NIST Webbook
tb	744.81	K	Joback Method
tc	930.58	K	Joback Method
tf	441.60	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.17	J/mol×K	744.81	Joback Method
cpg	748.32	J/mol×K	775.77	Joback Method
cpg	762.52	J/mol×K	806.73	Joback Method
cpg	775.80	J/mol×K	837.70	Joback Method
cpg	788.17	J/mol×K	868.66	Joback Method
cpg	799.66	J/mol×K	899.62	Joback Method
cpg	810.29	J/mol×K	930.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405499&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