Glutaric acid, 1,1,1-trifluoroprop-2-yl (2-naphthyl)methyl ester

Inchi: InChI=1S/C19H19F3O4/c1-13(19(20,21)22)26-18(24)8-4-7-17(23)25-12-14-9-10-15-5-2-

InchiKey: XZAJGHIHCPUVPJ-UHFFFAOYSA-N

Formula: C19H19F3O4

SMILES: CC(OC(=O)CCCC(=O)OCc1ccc2ccccc2c1)C(F)(F)F

Mol. weight [g/mol]: 368.35

Physical Properties

Property code	Value	Unit	Source
gf	-733.34	kJ/mol	Joback Method
hf	-1111.32	kJ/mol	Joback Method
hfus	39.51	kJ/mol	Joback Method
hvap	76.64	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.547		Crippen Method
mcvol	255.540	ml/mol	McGowan Method
pc	1603.85	kPa	Joback Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook
tb	831.48	K	Joback Method
tc	1038.31	K	Joback Method
tf	509.04	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.79	J/mol×K	831.48	Joback Method
cpg	782.94	J/mol×K	865.95	Joback Method
cpg	795.13	J/mol×K	900.42	Joback Method
cpg	806.41	J/mol×K	934.89	Joback Method
cpg	816.84	J/mol×K	969.36	Joback Method
cpg	826.50	J/mol×K	1003.84	Joback Method
cpg	835.44	J/mol×K	1038.31	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=U392192&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