Glutaric acid, 1,1,1-trifluoroprop-2-yl 1-naphthyl ester

Inchi: InChI=1S/C18H17F3O4/c1-12(18(19,20)21)24-16(22)10-5-11-17(23)25-15-9-4-7-13-6-2-

InchiKey: LXFCABFOAAXFTE-UHFFFAOYSA-N

Formula: C18H17F3O4

SMILES: CC(OC(=O)CCCC(=O)Oc1cccc2ccccc12)C(F)(F)F

Mol. weight [g/mol]: 354.32

Physical Properties

Property code	Value	Unit	Source
gf	-741.76	kJ/mol	Joback Method
hf	-1090.68	kJ/mol	Joback Method
hfus	36.92	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.410		Crippen Method
mcvol	241.450	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
tb	808.60	K	Joback Method
tc	1016.26	K	Joback Method
tf	497.77	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.86	J/mol×K	808.60	Joback Method
cpg	726.73	J/mol×K	843.21	Joback Method
cpg	738.63	J/mol×K	877.82	Joback Method
cpg	749.63	J/mol×K	912.43	Joback Method
cpg	759.80	J/mol×K	947.04	Joback Method
cpg	769.19	J/mol×K	981.65	Joback Method
cpg	777.86	J/mol×K	1016.26	Joback Method

Sources

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=U393325&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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