Glutaric acid, 2,2,3,3-tetrafluoropropyl 1-naphthyl ester

Inchi: InChI=1S/C18H16F4O4/c19-17(20)18(21,22)11-25-15(23)9-4-10-16(24)26-14-8-3-6-12-5

InchiKey: WMECHDQUGGDXDL-UHFFFAOYSA-N

Formula: C18H16F4O4

SMILES: O=C(CCCC(=O)Oc1cccc2ccccc12)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 372.31

Physical Properties

Property code	Value	Unit	Source
gf	-936.57	kJ/mol	Joback Method
hf	-1286.79	kJ/mol	Joback Method
hfus	40.00	kJ/mol	Joback Method
hvap	73.60	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.359		Crippen Method
mcvol	243.220	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpol	2315.00		NIST Webbook
rinpol	2315.00		NIST Webbook
tb	807.87	K	Joback Method
tc	1009.79	K	Joback Method
tf	498.36	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.44	J/mol×K	807.87	Joback Method
cpg	733.85	J/mol×K	841.52	Joback Method
cpg	745.35	J/mol×K	875.18	Joback Method
cpg	755.98	J/mol×K	908.83	Joback Method
cpg	765.82	J/mol×K	942.48	Joback Method
cpg	774.92	J/mol×K	976.14	Joback Method
cpg	783.32	J/mol×K	1009.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393326&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