Glutaric acid, 1,1,1-trifluoroprop-2-yl 2,4-dichloro-1-naphthyl ester

Inchi: InChI=1S/C18H15Cl2F3O4/c1-10(18(21,22)23)26-15(24)7-4-8-16(25)27-17-12-6-3-2-5-1

InchiKey: LESXNJNSYIKHSA-UHFFFAOYSA-N

Formula: C18H15Cl2F3O4

SMILES: CC(OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12)C(F)(F)F

Mol. weight [g/mol]: 423.21

Physical Properties

Property code	Value	Unit	Source
gf	-784.88	kJ/mol	Joback Method
hf	-1145.10	kJ/mol	Joback Method
hfus	44.54	kJ/mol	Joback Method
hvap	84.51	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	5.716		Crippen Method
mcvol	265.930	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
tb	893.42	K	Joback Method
tc	1110.92	K	Joback Method
tf	582.65	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.69	J/mol×K	893.42	Joback Method
cpg	766.26	J/mol×K	929.67	Joback Method
cpg	775.96	J/mol×K	965.92	Joback Method
cpg	784.84	J/mol×K	1002.17	Joback Method
cpg	792.98	J/mol×K	1038.42	Joback Method
cpg	800.42	J/mol×K	1074.67	Joback Method
cpg	807.23	J/mol×K	1110.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392013&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume