Glutaric acid, 1,1,1-trifluoroprop-2-yl 4-cyanophenyl ester

Inchi: InChI=1S/C15H14F3NO4/c1-10(15(16,17)18)22-13(20)3-2-4-14(21)23-12-7-5-11(9-19)6-

InchiKey: REESAFQZGUNGSO-UHFFFAOYSA-N

Formula: C15H14F3NO4

SMILES: CC(OC(=O)CCCC(=O)Oc1ccc(C#N)cc1)C(F)(F)F

Mol. weight [g/mol]: 329.27

Physical Properties

Property code	Value	Unit	Source
gf	-740.49	kJ/mol	Joback Method
hf	-1054.95	kJ/mol	Joback Method
hfus	33.64	kJ/mol	Joback Method
hvap	76.58	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.128		Crippen Method
mcvol	220.020	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2023.00		NIST Webbook
rinpol	2023.00		NIST Webbook
tb	823.06	K	Joback Method
tc	1030.55	K	Joback Method
tf	496.25	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.88	J/mol×K	823.06	Joback Method
cpg	651.55	J/mol×K	857.64	Joback Method
cpg	661.33	J/mol×K	892.22	Joback Method
cpg	670.24	J/mol×K	926.80	Joback Method
cpg	678.31	J/mol×K	961.39	Joback Method
cpg	685.57	J/mol×K	995.97	Joback Method
cpg	692.05	J/mol×K	1030.55	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=U393270&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