Glutaric acid, naphth-2-ylmethyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C23H18F4O4/c24-22-18(23(25,26)27)7-3-8-19(22)31-21(29)10-4-9-20(28)30-1

InchiKey: GWBBYJZNBVYCBS-UHFFFAOYSA-N

Formula: C23H18F4O4

SMILES: O=C(CCCC(=O)Oc1cccc(C(F)(F)F)c1F)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 434.38

Physical Properties

Property code	Value	Unit	Source
gf	-798.88	kJ/mol	Joback Method
hf	-1171.12	kJ/mol	Joback Method
hfus	49.74	kJ/mol	Joback Method
hvap	88.72	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	5.817		Crippen Method
mcvol	289.910	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
tb	959.35	K	Joback Method
tc	1183.42	K	Joback Method
tf	621.17	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.29	J/mol×K	959.35	Joback Method
cpg	912.78	J/mol×K	996.69	Joback Method
cpg	923.31	J/mol×K	1034.04	Joback Method
cpg	932.96	J/mol×K	1071.38	Joback Method
cpg	941.82	J/mol×K	1108.73	Joback Method
cpg	949.99	J/mol×K	1146.07	Joback Method
cpg	957.54	J/mol×K	1183.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393629&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