Glutaric acid, 2-ethylhexyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C20H26F4O4/c1-3-5-8-14(4-2)13-27-17(25)11-7-12-18(26)28-16-10-6-9-15(19

InchiKey: QLAKVOVQAZRGPI-UHFFFAOYSA-N

Formula: C20H26F4O4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 406.41

Physical Properties

Property code	Value	Unit	Source
gf	-1036.01	kJ/mol	Joback Method
hf	-1530.61	kJ/mol	Joback Method
hfus	47.78	kJ/mol	Joback Method
hvap	77.07	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.680		Crippen Method
mcvol	290.860	ml/mol	McGowan Method
pc	1190.70	kPa	Joback Method
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
tb	839.63	K	Joback Method
tc	1032.27	K	Joback Method
tf	500.72	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.10	J/mol×K	839.63	Joback Method
cpg	922.87	J/mol×K	871.74	Joback Method
cpg	936.60	J/mol×K	903.84	Joback Method
cpg	949.33	J/mol×K	935.95	Joback Method
cpg	961.09	J/mol×K	968.06	Joback Method
cpg	971.92	J/mol×K	1000.16	Joback Method
cpg	981.85	J/mol×K	1032.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393621&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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