Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-heptyl ester

Inchi: InChI=1S/C15H25F3O4/c1-4-5-6-8-11(2)21-13(19)9-7-10-14(20)22-12(3)15(16,17)18/h1

InchiKey: SSYQKEQPYTWDED-UHFFFAOYSA-N

Formula: C15H25F3O4

SMILES: CCCCCC(C)OC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 326.35

Physical Properties

Property code	Value	Unit	Source
gf	-978.89	kJ/mol	Joback Method
hf	-1450.17	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	62.77	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.163		Crippen Method
mcvol	242.400	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	688.88	K	Joback Method
tc	859.96	K	Joback Method
tf	377.32	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.11	J/mol×K	688.88	Joback Method
cpg	719.49	J/mol×K	717.39	Joback Method
cpg	734.07	J/mol×K	745.91	Joback Method
cpg	747.89	J/mol×K	774.42	Joback Method
cpg	760.95	J/mol×K	802.94	Joback Method
cpg	773.27	J/mol×K	831.45	Joback Method
cpg	784.87	J/mol×K	859.96	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=U393576&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