Glutaric acid, hept-2-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C15H23F5O4/c1-3-4-5-7-11(2)24-13(22)9-6-8-12(21)23-10-14(16,17)15(18,19)

InchiKey: QGNGGVORWKOZGN-UHFFFAOYSA-N

Formula: C15H23F5O4

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

Mol. weight [g/mol]: 362.33

Physical Properties

Property code	Value	Unit	Source
gf	-1363.23	kJ/mol	Joback Method
hf	-1845.86	kJ/mol	Joback Method
hfus	37.23	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.409		Crippen Method
mcvol	245.940	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	1504.00		NIST Webbook
rinpol	1504.00		NIST Webbook
tb	684.63	K	Joback Method
tc	850.37	K	Joback Method
tf	395.92	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.80	J/mol×K	684.63	Joback Method
cpg	736.39	J/mol×K	712.25	Joback Method
cpg	750.21	J/mol×K	739.88	Joback Method
cpg	763.27	J/mol×K	767.50	Joback Method
cpg	775.61	J/mol×K	795.12	Joback Method
cpg	787.25	J/mol×K	822.74	Joback Method
cpg	798.21	J/mol×K	850.37	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=U393671&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