Glutaric acid, hept-2-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C16H24F6O4/c1-3-4-5-7-11(2)26-13(24)9-6-8-12(23)25-10-15(18,19)14(17)16

InchiKey: FDLCYYMCNAIKID-UHFFFAOYSA-N

Formula: C16H24F6O4

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

Mol. weight [g/mol]: 394.35

Physical Properties

Property code	Value	Unit	Source
gf	-1552.06	kJ/mol	Joback Method
hf	-2067.89	kJ/mol	Joback Method
hfus	39.38	kJ/mol	Joback Method
hvap	61.25	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.748		Crippen Method
mcvol	261.800	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook
tb	706.34	K	Joback Method
tc	871.71	K	Joback Method
tf	392.78	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.51	J/mol×K	706.34	Joback Method
cpg	800.36	J/mol×K	733.90	Joback Method
cpg	814.40	J/mol×K	761.46	Joback Method
cpg	827.65	J/mol×K	789.02	Joback Method
cpg	840.16	J/mol×K	816.59	Joback Method
cpg	851.93	J/mol×K	844.15	Joback Method
cpg	863.01	J/mol×K	871.71	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=U393688&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