Glutaric acid, 2-methylpent-3-yl pentafluorobenzyl ester

Inchi: InChI=1S/C18H21F5O4/c1-4-11(9(2)3)27-13(25)7-5-6-12(24)26-8-10-14(19)16(21)18(23

InchiKey: URIIEMYFNQMNHZ-UHFFFAOYSA-N

Formula: C18H21F5O4

SMILES: CCC(OC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F)C(C)C

Mol. weight [g/mol]: 396.35

Physical Properties

Property code	Value	Unit	Source
gf	-1281.83	kJ/mol	Joback Method
hf	-1716.38	kJ/mol	Joback Method
hfus	48.40	kJ/mol	Joback Method
hvap	74.70	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.573		Crippen Method
mcvol	264.450	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
tb	810.87	K	Joback Method
tc	997.43	K	Joback Method
tf	498.91	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.84	J/mol×K	810.87	Joback Method
cpg	810.48	J/mol×K	841.96	Joback Method
cpg	823.20	J/mol×K	873.06	Joback Method
cpg	835.02	J/mol×K	904.15	Joback Method
cpg	845.92	J/mol×K	935.24	Joback Method
cpg	855.91	J/mol×K	966.33	Joback Method
cpg	864.99	J/mol×K	997.43	Joback Method

Sources

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=U391929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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