Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl (2-naphthyl)methyl ester

Inchi: InChI=1S/C21H18F8O4/c22-18(23)20(26,27)21(28,29)19(24,25)12-33-17(31)7-3-6-16(30

InchiKey: WQRSPADQHSGMPZ-UHFFFAOYSA-N

Formula: C21H18F8O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 486.35

Physical Properties

Property code	Value	Unit	Source
gf	-1684.87	kJ/mol	Joback Method
hf	-2150.65	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	5.768		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
pc	1208.99	kPa	Joback Method
rinpol	2487.00		NIST Webbook
tb	867.13	K	Joback Method
tc	1065.25	K	Joback Method
tf	539.37	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.84	J/mol×K	867.13	Joback Method
cpg	934.98	J/mol×K	900.15	Joback Method
cpg	946.27	J/mol×K	933.17	Joback Method
cpg	956.81	J/mol×K	966.19	Joback Method
cpg	966.70	J/mol×K	999.21	Joback Method
cpg	976.05	J/mol×K	1032.23	Joback Method
cpg	984.94	J/mol×K	1065.25	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=U392194&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