Glutaric acid, 2-ethylhexyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C16H25F5O4/c1-3-5-7-12(4-2)10-24-13(22)8-6-9-14(23)25-11-15(17,18)16(19

InchiKey: QPPAVUIMGNLHKH-UHFFFAOYSA-N

Formula: C16H25F5O4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 376.36

Physical Properties

Property code	Value	Unit	Source
gf	-1354.81	kJ/mol	Joback Method
hf	-1866.50	kJ/mol	Joback Method
hfus	39.82	kJ/mol	Joback Method
hvap	62.46	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.657		Crippen Method
mcvol	260.030	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
tb	707.51	K	Joback Method
tc	874.73	K	Joback Method
tf	407.19	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.23	J/mol×K	707.51	Joback Method
cpg	792.28	J/mol×K	735.38	Joback Method
cpg	806.51	J/mol×K	763.25	Joback Method
cpg	819.96	J/mol×K	791.12	Joback Method
cpg	832.65	J/mol×K	818.99	Joback Method
cpg	844.61	J/mol×K	846.86	Joback Method
cpg	855.88	J/mol×K	874.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U393673&Units=SI

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