Glutaric acid, 2-ethylhexyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C17H26F6O4/c1-3-5-7-12(4-2)10-26-13(24)8-6-9-14(25)27-11-16(19,20)15(18

InchiKey: VWYDICWQKUBICZ-UHFFFAOYSA-N

Formula: C17H26F6O4

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

Mol. weight [g/mol]: 408.38

Physical Properties

Property code	Value	Unit	Source
gf	-1543.64	kJ/mol	Joback Method
hf	-2088.53	kJ/mol	Joback Method
hfus	41.97	kJ/mol	Joback Method
hvap	63.48	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.995		Crippen Method
mcvol	275.890	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	1757.00		NIST Webbook
rinpol	1757.00		NIST Webbook
tb	729.22	K	Joback Method
tc	896.96	K	Joback Method
tf	404.05	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.95	J/mol×K	729.22	Joback Method
cpg	857.27	J/mol×K	757.18	Joback Method
cpg	871.73	J/mol×K	785.13	Joback Method
cpg	885.38	J/mol×K	813.09	Joback Method
cpg	898.23	J/mol×K	841.05	Joback Method
cpg	910.33	J/mol×K	869.01	Joback Method
cpg	921.70	J/mol×K	896.96	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=U393690&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

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