

Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-ethylphenyl ester

Inchi:	InChI=1S/C18H18F8O4/c1-2-11-5-3-6-12(9-11)30-14(28)8-4-7-13(27)29-10-16(21,22)18
InchiKey:	KVISUVXQSMLPLZ-UHFFFAOYSA-N
Formula:	C18H18F8O4
SMILES:	CCc1cccc(OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F)c1
Mol. weight [g/mol]:	450.32

Physical Properties

Property code	Value	Unit	Source
gf	-1816.78	kJ/mol	Joback Method
hf	-2279.80	kJ/mol	Joback Method
hfus	40.48	kJ/mol	Joback Method
hvap	66.10	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.039		Crippen Method
mvol	269.760	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	1992.00		NIST Webbook
rinpol	1992.00		NIST Webbook
tb	779.51	K	Joback Method
tc	961.43	K	Joback Method
tf	472.86	K	Joback Method
vc	1.089	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.64	J/molxK	779.51	Joback Method
cpg	840.54	J/molxK	809.83	Joback Method
cpg	852.52	J/molxK	840.15	Joback Method
cpg	863.65	J/molxK	870.47	Joback Method
cpg	873.99	J/molxK	900.79	Joback Method
cpg	883.59	J/molxK	931.11	Joback Method
cpg	892.50	J/molxK	961.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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