Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl but-3-en-1-yl ester

Inchi: InChI=1S/C14H16F8O4/c1-2-3-7-25-9(23)5-4-6-10(24)26-8-12(17,18)14(21,22)13(19,20)

InchiKey: ZRBAXQGZHMOYKE-UHFFFAOYSA-N

Formula: C14H16F8O4

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

Mol. weight [g/mol]: 400.26

Physical Properties

Property code	Value	Unit	Source
gf	-1865.40	kJ/mol	Joback Method
hf	-2296.87	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	53.59	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.990		Crippen Method
mcvol	232.860	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	653.01	K	Joback Method
tc	811.49	K	Joback Method
tf	387.08	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.38	J/mol×K	653.01	Joback Method
cpg	684.11	J/mol×K	679.42	Joback Method
cpg	696.09	J/mol×K	705.84	Joback Method
cpg	707.37	J/mol×K	732.25	Joback Method
cpg	717.98	J/mol×K	758.66	Joback Method
cpg	727.95	J/mol×K	785.08	Joback Method
cpg	737.32	J/mol×K	811.49	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=U394031&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

Latest version available from:
https://www.chemeo.com/cid/117-065-0/Glutaric-acid-2-2-3-3-4-4-5-5-octafluoropentyl-but-3-en-1-yl-ester.pdf
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