Glutaric acid, 2,2,3,3-tetrafluoropropyl 3-octyl ester

Inchi: InChI=1S/C16H26F4O4/c1-3-5-6-8-12(4-2)24-14(22)10-7-9-13(21)23-11-16(19,20)15(17

InchiKey: SQCFWRMGXVBTID-UHFFFAOYSA-N

Formula: C16H26F4O4

SMILES: CCCCCC(CC)OC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 358.37

Physical Properties

Property code	Value	Unit	Source
gf	-1165.28	kJ/mol	Joback Method
hf	-1666.92	kJ/mol	Joback Method
hfus	40.63	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.502		Crippen Method
mcvol	258.260	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	1701.00		NIST Webbook
rinpol	1701.00		NIST Webbook
tb	711.03	K	Joback Method
tc	879.36	K	Joback Method
tf	389.18	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.73	J/mol×K	711.03	Joback Method
cpg	783.15	J/mol×K	739.08	Joback Method
cpg	797.76	J/mol×K	767.14	Joback Method
cpg	811.60	J/mol×K	795.19	Joback Method
cpg	824.66	J/mol×K	823.25	Joback Method
cpg	836.99	J/mol×K	851.30	Joback Method
cpg	848.59	J/mol×K	879.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391553&Units=SI
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

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