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

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

InchiKey: GFUNFVRTNLNJAS-UHFFFAOYSA-N

Formula: C16H26F4O4

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

Mol. weight [g/mol]: 358.37

Physical Properties

Property code	Value	Unit	Source
gf	-1162.84	kJ/mol	Joback Method
hf	-1661.64	kJ/mol	Joback Method
hfus	44.15	kJ/mol	Joback Method
hvap	64.57	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.504		Crippen Method
mcvol	258.260	ml/mol	McGowan Method
pc	1261.95	kPa	Joback Method
rinpol	1845.00		NIST Webbook
rinpol	1845.00		NIST Webbook
tb	711.47	K	Joback Method
tc	878.52	K	Joback Method
tf	404.18	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.24	J/mol×K	711.47	Joback Method
cpg	782.52	J/mol×K	739.31	Joback Method
cpg	797.02	J/mol×K	767.15	Joback Method
cpg	810.75	J/mol×K	794.99	Joback Method
cpg	823.73	J/mol×K	822.84	Joback Method
cpg	835.99	J/mol×K	850.68	Joback Method
cpg	847.54	J/mol×K	878.52	Joback Method

Sources

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=U391506&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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