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

Inchi: InChI=1S/C15H24F4O4/c1-3-4-5-7-11(2)23-13(21)9-6-8-12(20)22-10-15(18,19)14(16)17
InchiKey: XHFUKCHICXUSPM-UHFFFAOYSA-N
Formula: C15H24F4O4
SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 344.34

Physical Properties

Property code	Value	Unit	Source
gf	-1173.70	kJ/mol	Joback Method
hf	-1646.28	kJ/mol	Joback Method
hfus	38.04	kJ/mol	Joback Method
hvap	61.96	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.112		Crippen Method
mcvol	244.170	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	1633.00		NIST Webbook
rinpol	1633.00		NIST Webbook
tb	688.15	K	Joback Method
tc	855.06	K	Joback Method
tf	377.91	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.96	J/mol×K	688.15	Joback Method
cpg	726.91	J/mol×K	715.97	Joback Method
cpg	741.10	J/mol×K	743.79	Joback Method
cpg	754.55	J/mol×K	771.61	Joback Method
cpg	767.27	J/mol×K	799.43	Joback Method
cpg	779.28	J/mol×K	827.24	Joback Method
cpg	790.60	J/mol×K	855.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393577&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