

Glutaric acid, 3,3,4,4-tetrafluoropropyl hept-4-yl ester

Inchi:	InChI=1S/C15H24F4O4/c1-3-6-11(7-4-2)23-13(21)9-5-8-12(20)22-10-15(18,19)14(16)17
InchiKey:	LFJNBSKPMYDAGJ-UHFFFAOYSA-N
Formula:	C15H24F4O4
SMILES:	CCCC(CCC)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
mvol	244.170	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
tb	688.15	K	Joback Method
tc	855.06	K	Joback Method
tf	377.91	K	Joback Method
vc	0.973	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.96	J/molxK	688.15	Joback Method
cpg	726.91	J/molxK	715.97	Joback Method
cpg	741.10	J/molxK	743.79	Joback Method
cpg	754.55	J/molxK	771.61	Joback Method
cpg	767.27	J/molxK	799.43	Joback Method
cpg	779.28	J/molxK	827.24	Joback Method
cpg	790.60	J/molxK	855.06	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=U392508&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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