

Glutaric acid, 3-methylbut-2-enyl pentyl ester

Inchi:	InChI=1S/C15H26O4/c1-4-5-6-11-18-14(16)8-7-9-15(17)19-12-10-13(2)3/h10H,4-9,11-12
InchiKey:	KNPAAUCSSPQEBZ-UHFFFAOYSA-N
Formula:	C15H26O4
SMILES:	CCCCCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-320.75	kJ/mol	Joback Method
hf	-735.10	kJ/mol	Joback Method
hfus	39.07	kJ/mol	Joback Method
hvap	67.33	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.399		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpola	1904.00		NIST Webbook
rinpola	1904.00		NIST Webbook
tb	699.22	K	Joback Method
tc	881.91	K	Joback Method
tf	384.09	K	Joback Method
vc	0.904	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.34	J/molxK	699.22	Joback Method
cpg	670.11	J/molxK	729.67	Joback Method
cpg	685.10	J/molxK	760.12	Joback Method
cpg	699.32	J/molxK	790.57	Joback Method
cpg	712.77	J/molxK	821.02	Joback Method
cpg	725.49	J/molxK	851.47	Joback Method
cpg	737.48	J/molxK	881.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360088&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
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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