

Glutaric acid, butyl trans-hex-3-enyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H26O4/c1-3-5-7-8-13-19-15(17)11-9-10-14(16)18-12-6-4-2/h5,7H,3-4,6,8-1

YAZJWXLXRBNZES-FNORWQNLSA-N

C15H26O4

CCC=CCCOC(=O)CCCC(=O)OCCCC

270.36

Physical Properties

Property code	Value	Unit	Source
gf	-312.20	kJ/mol	Joback Method
hf	-725.31	kJ/mol	Joback Method
hfus	40.38	kJ/mol	Joback Method
hvap	67.25	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.399		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook
tb	699.34	K	Joback Method
tc	880.04	K	Joback Method
tf	398.05	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.66	J/mol×K	699.34	Joback Method
cpg	725.18	J/mol×K	849.93	Joback Method
cpg	712.57	J/mol×K	819.81	Joback Method
cpg	699.22	J/mol×K	789.69	Joback Method
cpg	685.13	J/mol×K	759.57	Joback Method
cpg	670.28	J/mol×K	729.46	Joback Method
cpg	737.08	J/mol×K	880.04	Joback Method
dvisc	0.0000910	Pa×s	699.34	Joback Method

dvisc	0.0001192	Pa×s	649.12	Joback Method
dvisc	0.0001632	Pa×s	598.91	Joback Method
dvisc	0.0002368	Pa×s	548.69	Joback Method
dvisc	0.0003703	Pa×s	498.48	Joback Method
dvisc	0.0006402	Pa×s	448.26	Joback Method
dvisc	0.0012706	Pa×s	398.05	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=U359924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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