

Malonic acid, isoheptyl 3-methylpentyl ester

Inchi:	InChI=1S/C15H28O4/c1-5-13(4)8-10-19-15(17)11-14(16)18-9-6-7-12(2)3/h12-13H,5-11H
InchiKey:	MBNZHPZCFOUHTI-UHFFFAOYSA-N
Formula:	C15H28O4
SMILES:	CCC(C)CCOC(=O)CC(=O)OCCCC(C)C
Mol. weight [g/mol]:	272.38

Physical Properties

Property code	Value	Unit	Source
gf	-397.30	kJ/mol	Joback Method
hf	-853.09	kJ/mol	Joback Method
hfus	33.13	kJ/mol	Joback Method
hvap	66.52	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.335		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	1747.00		NIST Webbook
tb	694.30	K	Joback Method
tc	874.56	K	Joback Method
tf	373.13	K	Joback Method
vc	0.911	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.23	J/molxK	694.30	Joback Method
cpg	694.81	J/molxK	724.34	Joback Method
cpg	710.56	J/molxK	754.39	Joback Method
cpg	725.49	J/molxK	784.43	Joback Method
cpg	739.62	J/molxK	814.47	Joback Method
cpg	752.95	J/molxK	844.52	Joback Method
cpg	765.47	J/molxK	874.56	Joback Method
dvisc	0.0020958	Paxs	373.13	Joback Method
dvisc	0.0008937	Paxs	426.66	Joback Method

dvisc	0.0004608	Paxs	480.19	Joback Method
dvisc	0.0002714	Paxs	533.71	Joback Method
dvisc	0.0001760	Paxs	587.24	Joback Method
dvisc	0.0001227	Paxs	640.77	Joback Method
dvisc	0.0000905	Paxs	694.30	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=U348675&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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