

Adipic acid, «beta»-citronellyl heptyl ester

Inchi:	InChI=1S/C23H42O4/c1-5-6-7-8-11-18-26-22(24)15-9-10-16-23(25)27-19-17-21(4)14-12
InchiKey:	RJLFNEAKYPJHFV-UHFFFAOYSA-N
Formula:	C23H42O4
SMILES:	CCCCCCCOC(=O)CCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]:	382.58

Physical Properties

Property code	Value	Unit	Source
gf	-255.83	kJ/mol	Joback Method
hf	-905.50	kJ/mol	Joback Method
hfus	56.27	kJ/mol	Joback Method
hvap	84.75	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.376		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	935.77	kPa	Joback Method
rinpol	2576.00		NIST Webbook
tb	881.82	K	Joback Method
tc	1079.75	K	Joback Method
tf	459.25	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1127.93	J/molxK	881.82	Joback Method
cpg	1146.96	J/molxK	914.81	Joback Method
cpg	1164.79	J/molxK	947.80	Joback Method
cpg	1181.46	J/molxK	980.79	Joback Method
cpg	1197.00	J/molxK	1013.77	Joback Method
cpg	1211.45	J/molxK	1046.76	Joback Method
cpg	1224.86	J/molxK	1079.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353771&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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